

## Coordination Behavior of $[\text{Cp}^*_2\text{Zr}(\eta^{1:1}\text{-As}_4)]$ towards Different Lewis Acids

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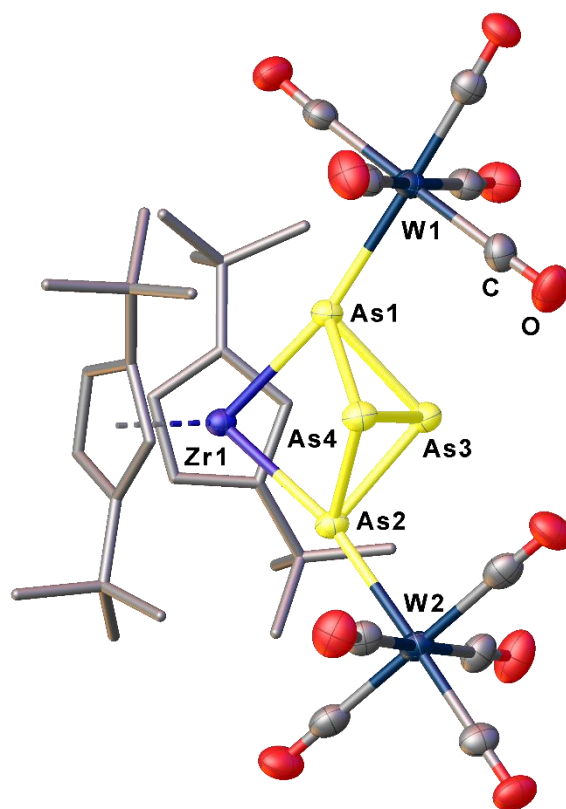
## 1. Crystallographic data

Crystals suitable for single crystal X-ray diffraction analysis were obtained as described above. The diffraction intensities were collected either on a Gemini Ultra diffractometer equipped with a Ruby or an Atlas<sup>S2</sup> CCD detector using Cu-K $\alpha$  radiation (fine-focus sealed X-ray tube) (**2**, **5**), at a XtaLAB Synergy R, DW system equipped with a HyPix-Arc 150 detector using Cu-K $\alpha$  radiation (rotating-anode) (**7**), a GV50 diffractometer equipped with a Titan<sup>S2</sup> CCD detector using Cu-K $\alpha$  or Cu-K $\beta$  radiation (micro-focus sealed X-ray tube) (**3**, **6a**, **6b**, **6c**) or at a SuperNova diffractometer equipped with an Atlas CCD detector using Cu-K $\alpha$  radiation (micro-focus sealed X-ray tube) (**4**). Data collection and reduction were performed with the **CrysAlisPro** software package (version 1.171.35.15 (**2**), 1.171.40.14a (**3**, **4**, **5**, **6c**); 1.171.40.18c (**6b**); 1.171.41.83a (**7**); 1.171.41.90a (**6a**)).<sup>[1]</sup> A numerical absorption correction based on gaussian integration over a multifaceted crystal model and an empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm, was performed for the compounds (**3**, **4**, **6b**, **6c**, **7**).<sup>[1]</sup> An analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R. C. Clark & J. S. Reid. (Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* A51, 887-897) and an empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm, was performed for compound (**5**).<sup>[1]</sup> A multi-scan absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm, was performed for the compounds (**2**, **6a**).<sup>[1]</sup> Using **Olex2**,<sup>[2]</sup> the structures were solved with **olex2.solve**<sup>[3]</sup> (**2**, **6b**, **7**) or **ShelXT**<sup>[4]</sup> (**3**, **4**, **5**, **6a**, **6c**) and refined by full-matrix least-squares method against  $|F|^2$  using **ShelXL**<sup>[4]</sup>. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms at the carbon atoms were located in idealized positions and refined with isotropic displacement parameters according to the riding model. Using **Olex2**,<sup>[2]</sup> all pictures of the respective molecular structures were made.

CCDC reference numbers 2077256 (**2**), 2077257 (**3**), 2077258 (**4**), 2077259 (**5**), 2077260 (**6a**), 2077261 (**6b**), 2077262 (**6c**) and 2077263 (**7**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html) (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: + 44-1223-336-033; e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)).

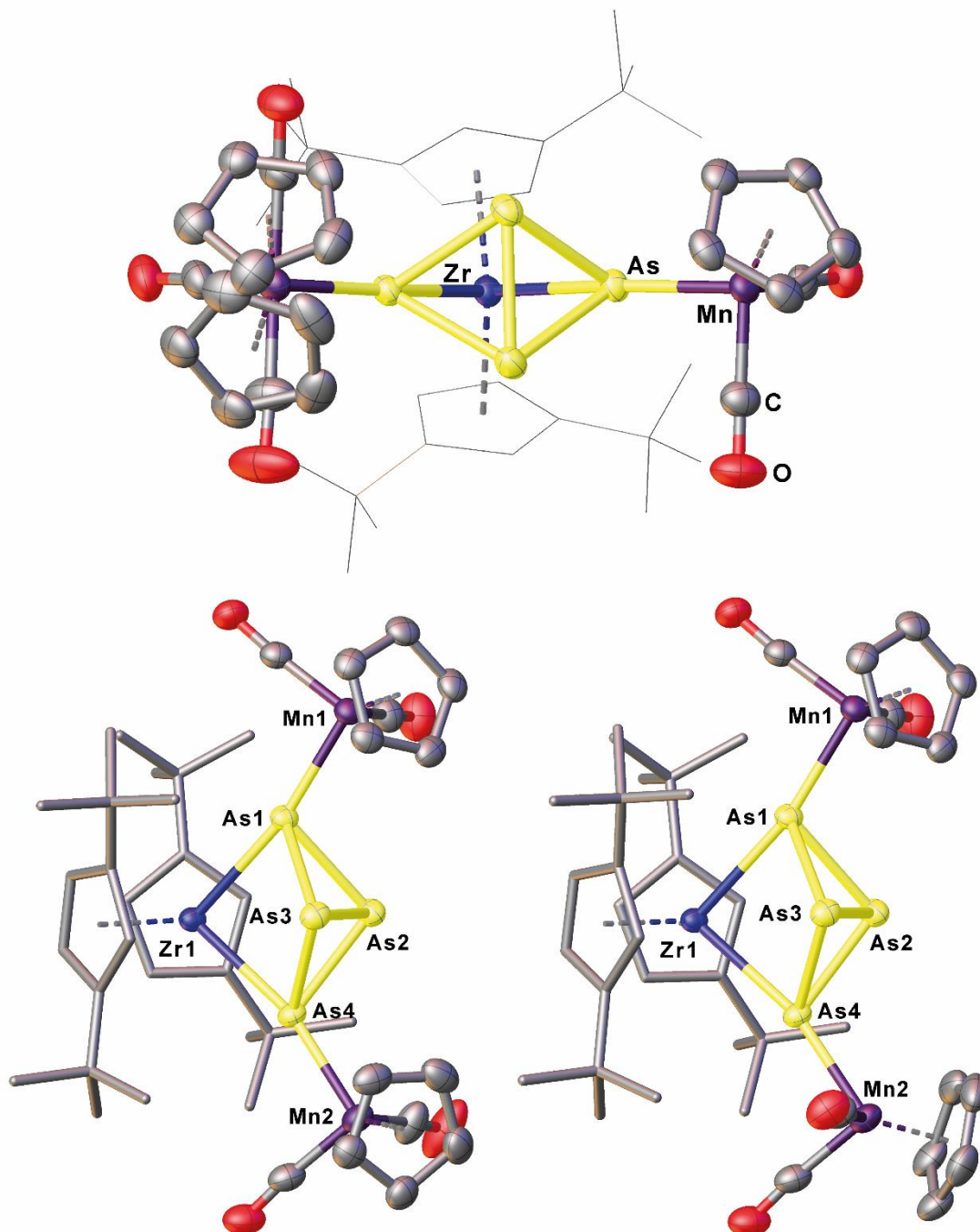
**[Cp<sup>''</sup>]<sub>2</sub>Zr(η<sup>1:1:1:1</sup>-As<sub>4</sub>)(W(CO)<sub>5</sub>)<sub>2</sub> (**2**):**

Compound **2** crystallizes out of a concentrated *n*-hexane solution at -78 °C in form of red blocks in the triclinic space group *P*-1. The asymmetric unit contains one molecule of **2**.



**Figure S1:** Molecular structure of **2** in the solid state. Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp<sup>''</sup> ligands are drawn in the tube model for clarity. Selected bond lengths [Å] and angles [°]: As1-As2 2.4575(6), As1-As3 2.4616(6), As1-W1 2.6460(4), As1-Zr1 2.7021(5), As2-As3 2.4363(6), As2-As4 2.4558(6), As3-As4 2.4649(6), As4-W2 2.6595(4), As4-Zr1 2.7008(5); As2-As1-As3 59.374(18), As2-As1-W1 104.814(19), As2-As1-Zr1 82.962(17), As3-As1-W1 107.84(2), As3-As1-Zr1 83.495(18), W1-As1-Zr1 168.38(2), As3-As2-As1 60.397(18), As3-As2-As4 60.508(18), As4-As2-As1 93.02(2), As1-As3-As4 92.70(2), As2-As3-As1 60.229(18), As2-As3-As4 60.139(18), As2-As4-As3 59.352(18), As2-As4-W2 107.436(19), As2-As4-Zr1 83.020(18), As3-As4-W2 106.51(2), As3-As4-Zr1 83.461(18), W2-As4-Zr 1168.14(2).

Compound **3** crystallizes out of a concentrated *n*-pentane solution at -78 °C in form of violet blocks in the triclinic space group  $P\bar{1}$ . The asymmetric unit contains one molecule of **3**. One [CpMn(CO)<sub>2</sub>] fragment is disordered over two positions (occupancy of 0.52 and 0.48).

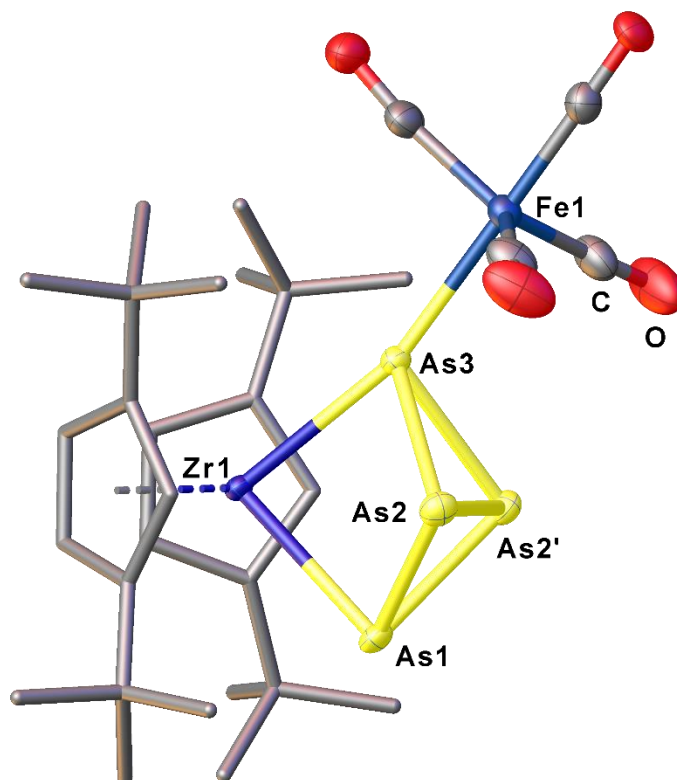


**Figure S2:** Molecular structure of **3** in the solid state (above). Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp'' ligands are drawn in the wireframe model for clarity. The separate parts of the disorder are depicted below (left: part1, occupancy of 52%; right: part2, occupancy of 48%). Hydrogen atoms are omitted and the Cp'' ligands are drawn in the tube model for clarity. Selected bond lengths [Å] and angles [°]: Zr1-As4 2.6874(3), Zr1-As1 2.6837(3), As4-As2 2.4726(4), As4-As3 2.4666(4), As4-Mn2 2.3732(5), As1-As2 2.4710(4), As1-As3 2.4699(4), As1-Mn1

2.3605(4), As2-As3 2.4394(4); As1-Zr1-As4 85.871(9), As2-As4-Zr1 80.039(11), As3-As4-Zr1 80.228(10), As3-As4-As2 59.193(11), Mn2-As4-Zr1 166.512(16), Mn2-As4-As2 112.664(16), Mn2-As4-As3 109.772(15), As2-As1-Zr1 80.139(11), As3-As1-Zr1 80.242(10), As3-As1-As2 59.170(11), Mn1-As1-Zr1 167.600(15), Mn1-As1-As2 108.773(15), Mn1-As1-As3 111.582(15), As1-As2-As4 95.477(13), As3-As2-As4 60.282(11), As3-As2-As1 60.393(11), As4-As3-As1 95.656(12), As2-As3-As4 60.525(11), As2-As3-As1 60.437(11).

**[Cp<sup>''</sup><sub>2</sub>Zr(μ,η<sup>1:1:1</sup>-As<sub>4</sub>)(Fe(CO)<sub>4</sub>)] (4):**

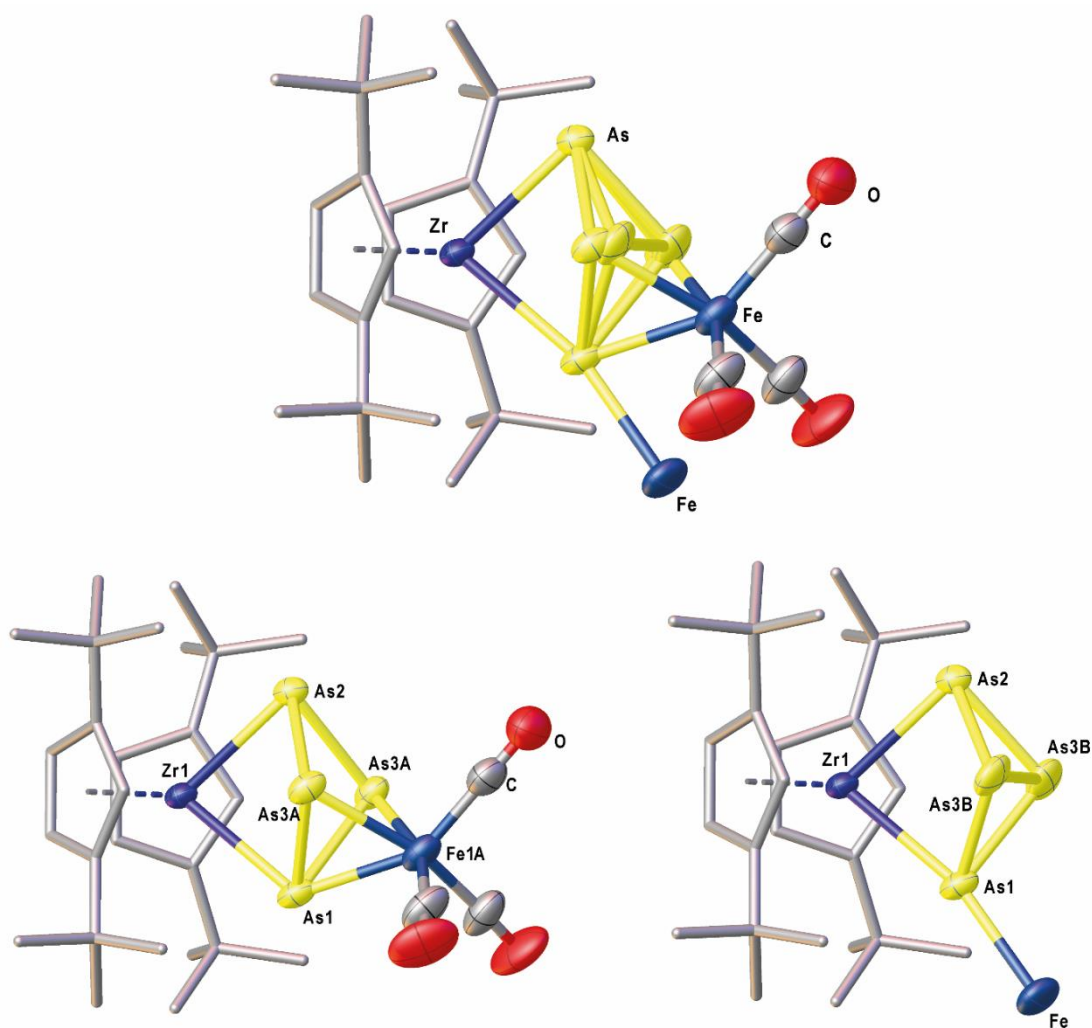
Compound **4** crystallizes out of a concentrated *n*-pentane solution at -78 °C in form of orange plates in the monoclinic space group *P*2<sub>1</sub>/*m*. The asymmetric unit contains half a molecule of **4**. One carbonyl ligand, which is located on a mirror plane, shows a disorder over three positions (occupancy of 0.6, 0.2 and 0.2). To describe the disorder the restraints ISOR and SIMU were used.



**Figure S3:** Molecular structure of **4** in the solid state. Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp<sup>''</sup> ligands are drawn in the tube model for clarity. Selected bond lengths [Å] and angles [°]: Zr1-As3 2.7078(4), Zr1-As1 2.6851(5), As3-As2 2.4791(4), As3-As2' 2.4791(4), As3-Fe1 2.4213(7), As1-As2 2.4457(4), As1-As2' 2.4457(4), As2-As2' 2.4321(6); As1-Zr1-As3 83.029(14), Fe1-As3-As2 110.125(19), Fe1-As3-As2' 110.125(19), As2'-As1-Zr1 83.508(13), As2-As1-Zr1 83.508(14), As2'-As1-As2 59.632(17), As1-As2-As3 93.072(14), As2'-As2-As3 60.626(8), As2'-As2-As1 60.184(8), As2'-As3-Zr1 82.416(13), As2-As3-Zr1 82.416(13), As2-As3-As2' 58.748(16), Fe1-As3-Zr1 165.46(2).

**[Cp''<sub>2</sub>Zr(μ,η<sup>3:1:1</sup>-As<sub>4</sub>)(Fe(CO)<sub>3</sub>)] (5):**

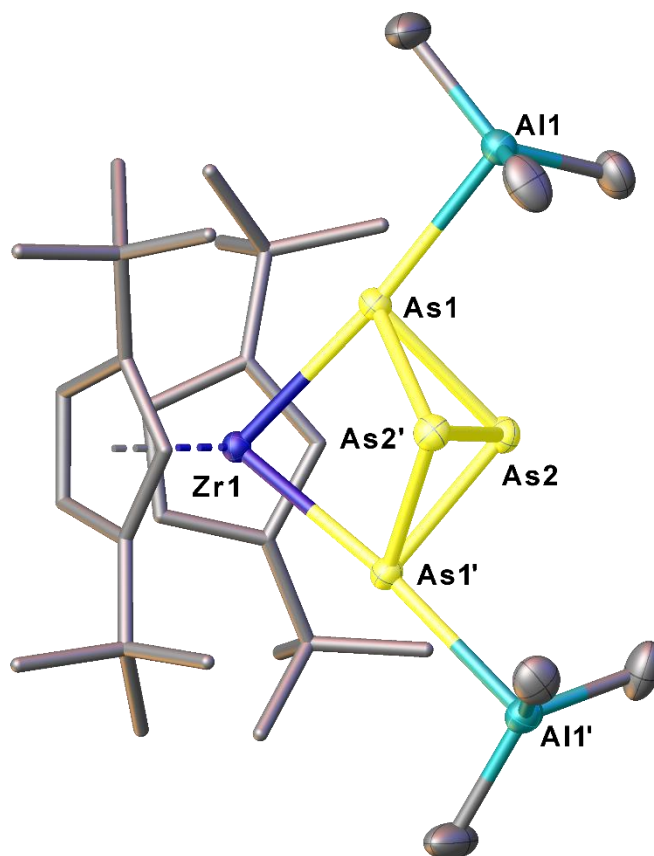
Compound **5** crystallizes out of a concentrated *n*-pentane solution at -78 °C in form of violet plates in the orthorhombic space group *Pnma*. The asymmetric unit contains half a molecule of **5** and an only partly occupied pentane solvent molecule. Due to heavy disorder it was not possible to model the pentane solvent molecule. Therefore, a solvent mask was calculated and 162 electrons were found in a volume of 756 Å<sup>3</sup> in 1 void per unit cell. This is consistent with the presence of 0.45 pentane molecules per asymmetric unit, which account for 151 electrons per unit cell. Further, compound **5** co-crystallizes with compound **4**. This co-crystallization is presented by the disorder of an As atom and a Fe(CO)<sub>4</sub> fragment (0.9 to 0.1). However, due to the low occupancy (0.1) and the disordered pentane molecule (overlapping positions) it was not possible to properly locate the CO ligands of the Fe(CO)<sub>4</sub> fragment.



**Figure S4:** Molecular structure of **5** in the solid state. Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp'' ligands are drawn in the wireframe model for clarity. Selected bond lengths [Å] and angles [°]: Zr1-As2 2.7105(8), Zr1-As1 2.7513(8), As2-As3A 2.4657(14), As2-As3B 2.377(14), As1-As3A 2.4721(13), As1-Fe1A 2.4265(15), As1-As3B 2.433(14), As3B-As3B' 2.391(18), As1-Fe1B 2.393(11), As3A-Fe1A 2.4151(16); As2-Zr1-As1 79.85(2), As3B'-As2-Zr1 84.9(4), As3A-As1-Zr1 78.54(4), As3A-As1-As3A' 75.65(7), Fe1A-As1-Zr1 124.84(4), Fe1A-As1-As3A 59.07(4), Fe1A-As1-As3B 50.4(3), As3B-As1-Zr1 82.9(4), As3B'-As1-As3B 58.9(5), Fe1B-As1-Zr1 165.8(3), Fe1B-As1-As3B 109.3(5), As2-As3A-As1 90.45(5), Fe1A-As3A-As2 99.36(5), Fe1A-As3A-As1 59.52(4), As3A-Fe1A-As1 61.40(4), As3A-Fe1A-As3A' 77.76(7), As2-As3B-As1 93.6(5), As2-As3B-As3B 59.8(2), As3B'-As3B-As1 60.6(2), As3A-As2-Zr1 79.44(4), As3A'-As2-As3A 75.88(6), As3B-As2-Zr1 84.9(4).

**[Cp''<sub>2</sub>Zr(μ<sub>3</sub>,η<sup>1:1:1:1</sup>-As<sub>4</sub>){AlMe<sub>3</sub>}<sub>2</sub>] (6a):**

Compound **6a** crystallizes out of a concentrated *n*-pentane solution at -30°C in form of orange blocks in the monoclinic space group *I*2/a. The asymmetric unit contains half a molecule of **6a**. The crystals of **6a** were twinned. Therefore, a refinement as a 2- component twin (BASF 0.57) was performed.

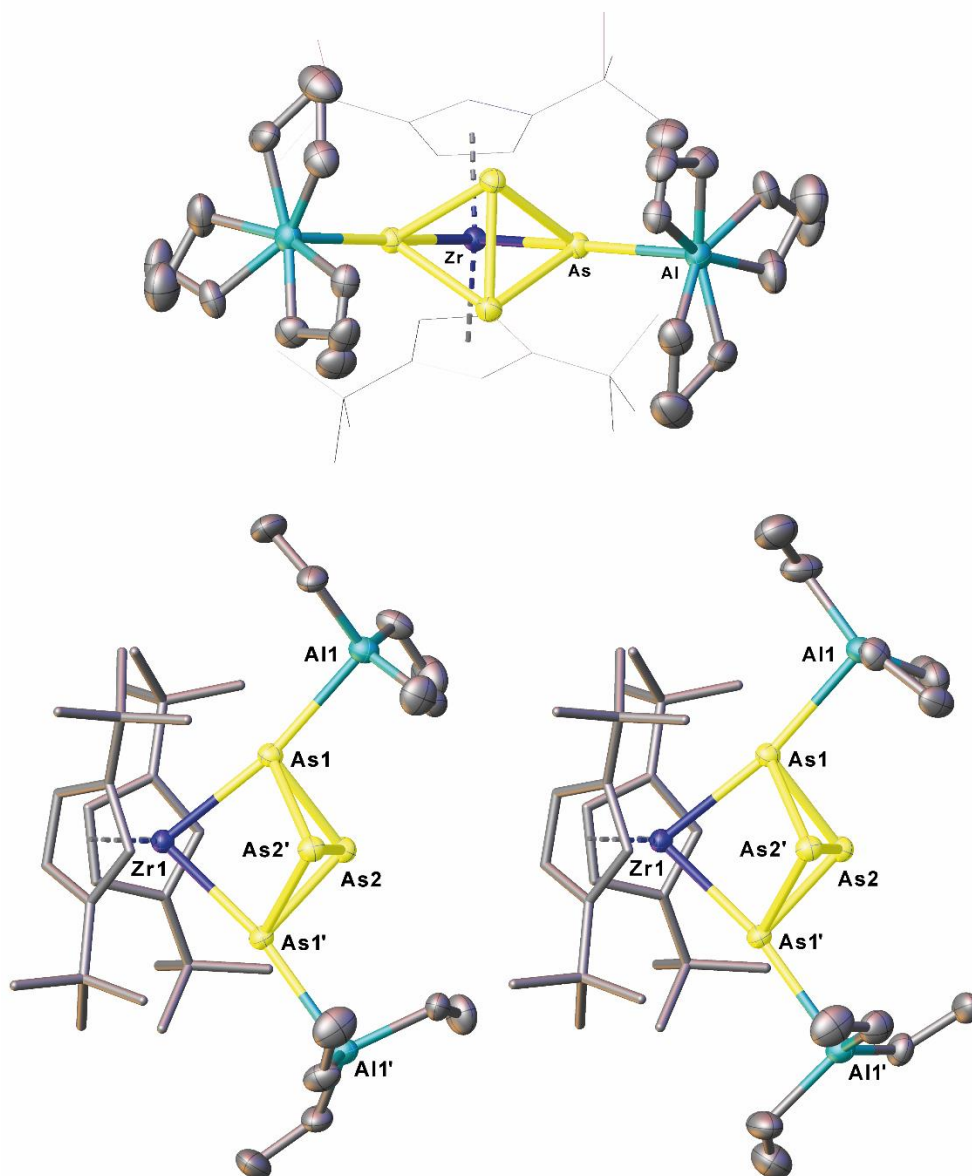


**Figure S5:** Molecular structure of **6a** in the solid state. Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp'' ligands are drawn in the tube model for clarity. Selected bond lengths [Å] and angles [°]: Zr1-As1' 2.6810(2), Zr1-As1 2.6810(2), As1-As2 2.4513(2), As1-As2'-2.4583(3), As1-Al1 2.6743(5), As2-As2' 2.4272(4); As1-Zr1-As1' 81.591(8), As2'-As1-Zr1 84.745(7), As2-As1-Zr1 84.881(7), As2-As1-As2' 59.258(9), As2-As1-Al1 100.118(13), As2'-As1-Al1 100.245(14), Al1-As1-Zr1 174.223(13), As1-As2-As1' 91.049(9), As2'-As2-As1' 60.225(8), As2'-As2-As1 60.515(8).



**[Cp''<sub>2</sub>Zr(μ<sub>3</sub>,η<sup>1:1:1:1</sup>-As<sub>4</sub>){AlEt<sub>3</sub>}<sub>2</sub>] (6b):**

Compound **6b** crystallizes out of a concentrated *n*-pentane solution at -30 °C in form of orange plates in the monoclinic space group *C2/c*. The asymmetric unit contains half a molecule of **6b**. The three ethyl substituents at AlEt<sub>3</sub> are disordered over two positions (occupancy 0.63:0.37; 0.63:0.37; 0.65:0.35). To describe the disorder of these ethyl substituents the restraints SADI and SIMU were used.

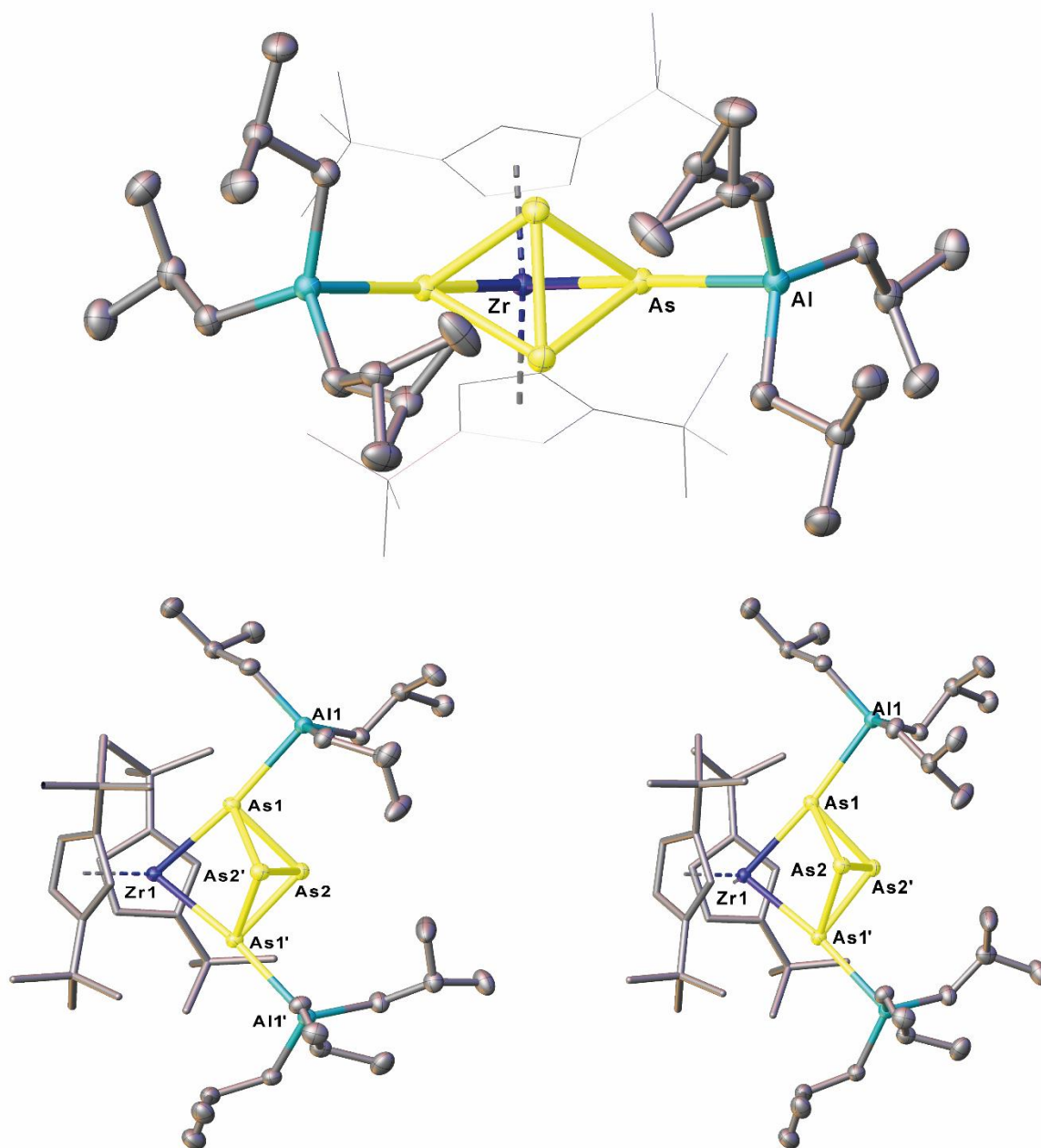


**Figure S6:** Molecular structure of **6b** in the solid state (above). Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp'' ligands are drawn in the wireframe model for clarity. The separate parts of the disorder are depicted below (left: part1, occupancy of 63%; right: part2, occupancy of 37%). Selected bond lengths [Å] and angles [°]: Zr1-As1 2.7018(2), Zr1-As1' 2.7019(2), As1-As2' 2.4637(2), As1-As2 2.4583(2), As1-Al1 2.7415(5), As2-As2' 2.4202(3); As1-Zr1-As1' 81.216(8), Zr1-As1-Al1 170.087(13), As2'-As1-Zr1 84.937(7), As2-As1-Zr1 85.042(6), As2-As1-As2' 58.907(8), As2-As1-Al1 102.934(13), As2'-As1-Al1 104.161(13), As1-As2-As1' 91.218(8), As2'-As2-As1' 60.435(7), As2'-As2-As1 60.658(7).



**[Cp''<sub>2</sub>Zr(μ<sub>3</sub>,η<sup>1:1:1:1</sup>-As<sub>4</sub>){Al<sup>i</sup>Bu<sub>3</sub>]<sub>2</sub>] (6c):**

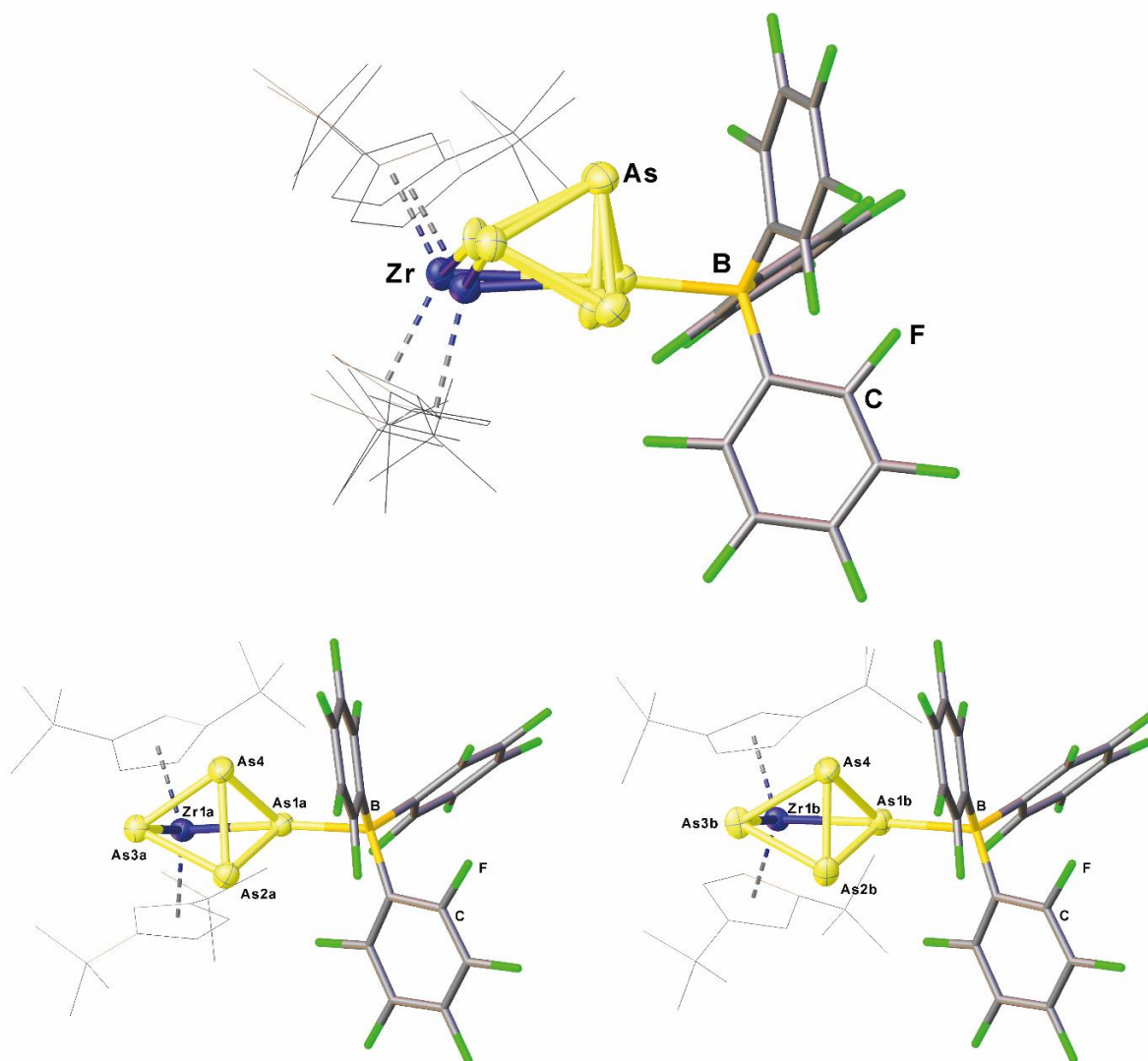
Compound **6c** crystallizes out of a concentrated *n*-pentane solution at -30 °C in form of orange blocks in the monoclinic space group *C2/c*. The asymmetric unit contains half a molecule of **6c**. A <sup>i</sup>Bu substituent of the Al<sup>i</sup>Bu<sub>3</sub> ligand is disordered over two positions (occupancy of 0.86 and 0.14). To describe the disorder the restraints SADI and SIMU were used.



**Figure S7:** Molecular structure of **6c** in the solid state (above). Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted and the Cp'' ligands are drawn in the wireframe model for clarity. The separate parts of the disorder are depicted below (left: part1, occupancy of 86%; right: part2, occupancy of 14%). Selected bond lengths [Å] and angles [°]: Zr1-As1' 2.6810(3), Zr1-As1 2.6810(3), As1-As2' 2.4696(3), As1-As2 2.4550(3), As1-Al1 2.7566(6), As2-As2' 2.4281(4); As1'-Zr1-As1 83.462(11), Zr1-As1-Al1 172.833(15), As2'-As1-Zr1 82.784(8), As2-As1-Zr1 83.057(9), As2-As1-As2' 59.081(11), As2'-As1-Al1 104.082(15), As2-As1-Al1 102.142(15), As1-As2-As1' 92.896(11), As2'-As2-As1' 60.159(9), As2'-As2-As1 60.760(10).

**[Cp''<sub>2</sub>Zr(μ,η<sup>1:1</sup>-As<sub>4</sub>)(B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>)] (7):**

Compound **7** crystallizes out of a concentrated *n*-hexane solution at -30 °C in form of clear orange blocks in the triclinic space group *P* $\bar{1}$ . The asymmetric unit contains one molecule of **7**. The [Cp''<sub>2</sub>Zr(μ,η<sup>1:1</sup>-As<sub>4</sub>)] fragment is disordered over two positions (occupancy of 0.77 and 0.23). To describe the disorder the restraints SADI, SIMU and ISOR were used.



**Figure S8:** Molecular structure of **7** in the solid state (above). Thermal ellipsoids are depicted at 50% probability level. Hydrogen atoms are omitted, the Cp'' ligands are drawn in the wireframe model and the [BC<sub>18</sub>F<sub>15</sub>] unit is drawn in the tube model for clarity. The separate parts of the disorder are depicted below (left: part1, occupancy of 77%; right: part2, occupancy of 23%). Selected bond lengths [Å] and angles [°]: As1A-As2A 2.457(4), As3A-As4 2.436(3), As3A-As2A 2.437(4), As4-As1A 2.445(3), As4-As2A 2.442(3), As4-As1B 2.552(9), As4-As2B 2.357(13), As4-As3B 2.543(12), As4-As3B 2.543(12), As1B-As2B 2.434(14), Zr1B-As1B 2.789(7), Zr1B-As3B 2.595(10), Zr1A-As3A 2.732(3), Zr1A-As1A 2.732(2), As1A-B1 2.177(6), B1-As1B 2.518(8); As1A-Zr1A-As3A 79.83(8), As2A-As3A-Zr1A 86.27(11), As2A-As4-As1A 60.36(10), As2A-As1A-Zr1A 85.89(10), As3A-As2A-As4 59.89(10), As3A-As2A-As1A 91.51(11), As3A-As4-As1A 91.85(9), As3A-As4-As2A 59.96(10), As4-As2A-As1A 59.87(10), As4-As1A-Zr1A 83.69(7), As4-As1A-As2A 59.76(10), As4-As3A-Zr1A 83.86(10), As4-As3A-As2A 60.15(11), As2B-As4-As1B 59.3(3), As2B-As4-As3B 59.5(4), As3B-As4-As1B 85.3(3), As4-As1B-Zr1B 86.7(3), As2B-As1B-As4 56.4(4), As2B-As1B-B1 94.8(3), As2B-As1B-Zr1B 85.8(4), As4-As2B-As1B 64.4(4), As4-As2B-As3B 64.1(4), As1B-As2B-As3B 90.3(4), As4-As3B-Zr1B 91.2(4), As2B-As3B-As4 56.4(4), As2B-As3B-Zr1B 90.2(5), B1-As1B-As4 95.9(3), B1-As1A-As4 109.00(18), B1-As1A-As2A 101.90(17).

**Table S1:** Structure determination summary of the complexes **2**, **3** and **4**.

Compound	<b>2</b>	<b>3</b>	<b>4</b>
Formula	C <sub>36</sub> H <sub>42</sub> As <sub>4</sub> O <sub>10</sub> W <sub>2</sub> Zr	C <sub>40</sub> H <sub>52</sub> As <sub>4</sub> Mn <sub>2</sub> O <sub>4</sub> Zr	C <sub>30</sub> H <sub>42</sub> As <sub>4</sub> FeO <sub>4</sub> Zr
CCDC number	2077256	2077257	2077258
$D_{\text{calc.}}/\text{g cm}^{-3}$	2.151	1.752	1.764
$m/\text{mm}^{-1}$	15.466	7.938	10.399
Formula Weight	1393.29	1097.59	913.38
Colour	red	violet	clear light orange
Shape	block	block	plate
Size/mm <sup>3</sup>	0.15×0.07×0.03	0.25×0.19×0.10	0.27×0.19×0.09
$T/\text{K}$	123(1)	122.99(11)	123.01(10)
Crystal System	triclinic	triclinic	monoclinic
Space Group	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> / <i>m</i>
$a/\text{\AA}$	11.0989(3)	11.5684(3)	9.1335(2)
$b/\text{\AA}$	12.5065(3)	12.1340(4)	17.1283(3)
$c/\text{\AA}$	17.5582(5)	16.8248(4)	11.3330(2)
$\alpha/^\circ$	101.764(2)	80.103(2)	90
$\beta/^\circ$	95.394(2)	89.979(2)	104.114(2)
$\gamma/^\circ$	113.207(2)	63.838(2)	90
$V/\text{\AA}^3$	2151.41(10)	2080.60(11)	1719.43(6)
$Z$	2	2	2
$Z'$	1	1	0.5
Wavelength/ $\text{\AA}$	1.54178	1.39222	1.54184
Radiation type	CuK <sub><math>\alpha</math></sub>	Cu K <sub><math>\alpha</math></sub>	Cu K <sub><math>\alpha</math></sub>
$\theta_{\text{min}}/^\circ$	3.986	2.416	4.022
$\theta_{\text{max}}/^\circ$	66.565	74.751	72.087
Measured Refl's.	36658	46763	10794
Ind't Refl's	7562	11522	3482
Refl's with $I \geq \sigma(I)$	7021	10758	3418
$R_{\text{int}}$	0.0320	0.0415	0.0264
Parameters	490	535	217
Restraints	0	0	42
Largest Peak	1.615	0.806	1.429
Deepest Hole	-0.984	-1.049	-0.906
GooF	1.068	1.065	1.127
$wR_2$ (all data)	0.0730	0.0853	0.0670
$wR_2$	0.0711	0.0834	0.0666
$R_1$ (all data)	0.0297	0.0346	0.0259
$R_1$	0.0270	0.0323	0.0253

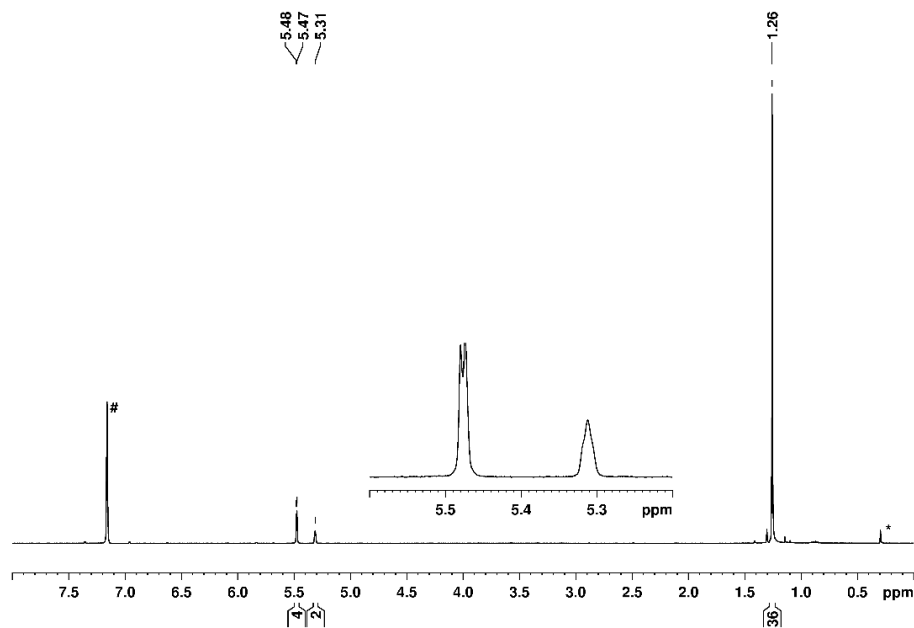
**Table S2:** Structure determination summary of the complexes **5**, **6a** and **6b**.

Compound	5	6a	6b
Formula	C <sub>33.2</sub> H <sub>52.8</sub> As <sub>4</sub> FeO <sub>2.7</sub> Zr	0.5·(C <sub>32</sub> H <sub>60</sub> Al <sub>2</sub> As <sub>4</sub> Zr)	0.5·(C <sub>38</sub> H <sub>72</sub> Al <sub>2</sub> As <sub>4</sub> Zr)
CCDC number	2077259	2077260	2077261
$D_{calc}/\text{g cm}^{-3}$	1.594	1.537	1.465
$m/\text{mm}^{-1}$	9.098	4.969	4.361
Formula Weight	941.90	889.66	973.81
Colour	dark violet	dark orange	orange
Shape	plate-shaped	block	plate
Size/mm <sup>3</sup>	0.25×0.20×0.14	0.20×0.11×0.08	0.25×0.21×0.12
$T/\text{K}$	123(1)	122.99(11)	123.00(11)
Crystal System	orthorhombic	monoclinic	monoclinic
Space Group	<i>Pnma</i>	<i>I2/a</i>	<i>C2/c</i>
$a/\text{\AA}$	12.0528(5)	17.6443(3)	25.1728(4)
$b/\text{\AA}$	17.2716(7)	9.95170(16)	10.3746(2)
$c/\text{\AA}$	18.8597(6)	23.1782(4)	18.0895(3)
$\alpha/^\circ$	90	90	90
$\beta/^\circ$	90	109.1757(19)	110.797(2)
$\gamma/^\circ$	90	90	90
$V/\text{\AA}^3$	3926.0(3)	3844.08(12)	4416.40(14)
$Z$	4	4	4
$Z'$	0.5	0.5	0.5
Wavelength/ $\text{\AA}$	1.54184	1.39222	1.39222
Radiation type	Cu K $\alpha$	Cu K	Cu K
$\theta_{min}/^\circ$	3.470	3.646	3.392
$\theta_{max}/^\circ$	71.632	74.104	74.810
Measured Refl's.	11708	9433	22870
Ind't Refl's	3893	9433	6087
Refl's with $I \geq \sigma(I)$	3256	8609	5789
$R_{int}$	0.0392	0.0752	0.0304
Parameters	202	188	264
Restraints	2	0	19
Largest Peak	1.294	1.497	0.806
Deepest Hole	-0.660	-0.897	-0.529
GooF	1.030	1.018	1.064
$wR_2$ (all data)	0.1108	0.1192	0.0631
$wR_2$	0.1051	0.1175	0.0620
$R_1$ (all data)	0.0501	0.0430	0.0256
$R_1$	0.0408	0.0407	0.0242

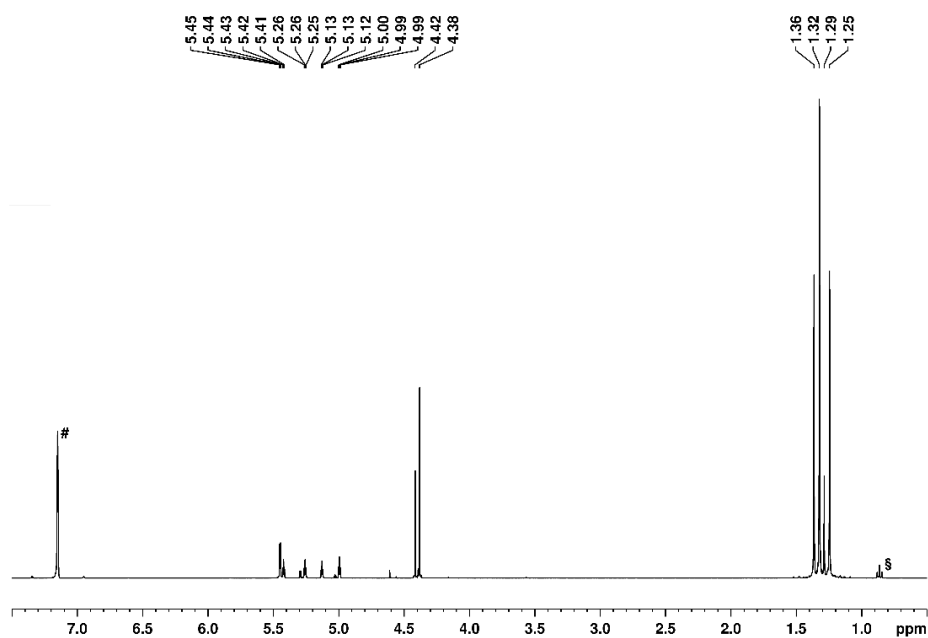
**Table S3:** Structure determination summary of the complexes **6c** and **7**.

Compound	<b>6c</b>	<b>7</b>
Formula	0.5·(C <sub>50</sub> H <sub>96</sub> Al <sub>2</sub> As <sub>4</sub> Zr)	C <sub>44</sub> H <sub>42</sub> As <sub>4</sub> BF <sub>15</sub> Zr
CCDC number	2077262	2077263
$D_{\text{calc.}}/\text{g cm}^{-3}$	1.343	1.823
$m/\text{mm}^{-1}$	3.465	6.020
Formula Weight	1142.12	1257.48
Colour	orange	clear orange
Shape	block	block
Size/mm <sup>3</sup>	0.22×0.17×0.10	0.21×0.14×0.11
$T/\text{K}$	123.00(10)	123.00(10)
Crystal System	monoclinic	triclinic
Space Group	<i>C</i> 2/ <i>c</i>	<i>P</i> -1
$a/\text{\AA}$	18.5668(4)	11.2797(4)
$b/\text{\AA}$	11.9157(2)	12.7421(5)
$c/\text{\AA}$	27.2938(5)	18.5702(6)
$\alpha/^\circ$	90	71.815(3)
$\beta/^\circ$	110.737(2)	87.410(3)
$\gamma/^\circ$	90	65.217(4)
$V/\text{\AA}^3$	5647.2(2)	2290.82(16)
$Z$	4	2
$Z'$	0.5	1
Wavelength/ $\text{\AA}$	1.39222	1.54184
Radiation type	Cu K $\alpha$	Cu K $\alpha$
$\theta_{\text{min}}/^\circ$	3.127	2.517
$\theta_{\text{max}}/^\circ$	64.688	73.366
Measured Refl's.	20223	28611
Ind't Refl's	6481	8705
Refl's with $I \geq \sigma(I)$	5866	7895
$R_{\text{int}}$	0.0282	0.0456
Parameters	280	880
Restraints	34	371
Largest Peak	0.804	0.610
Deepest Hole	-0.456	-0.814
GooF	1.049	1.136
$wR_2$ (all data)	0.0662	0.1158
$wR_2$	0.0642	0.1134
$R_1$ (all data)	0.0335	0.0502
$R_1$	0.0289	0.0457

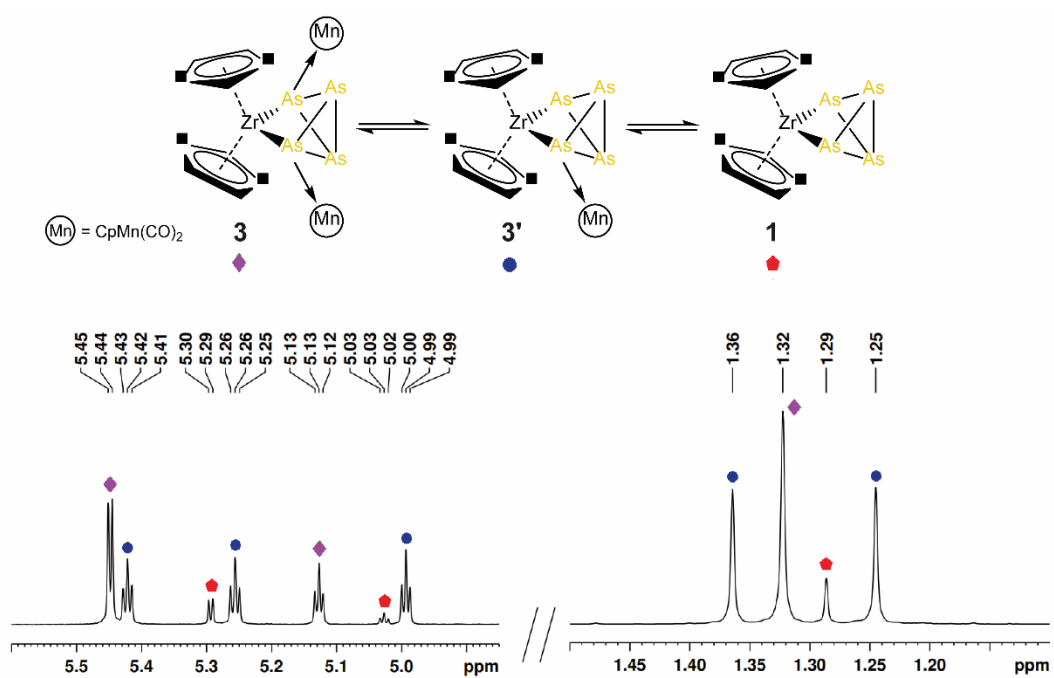
## 2. NMR Investigations



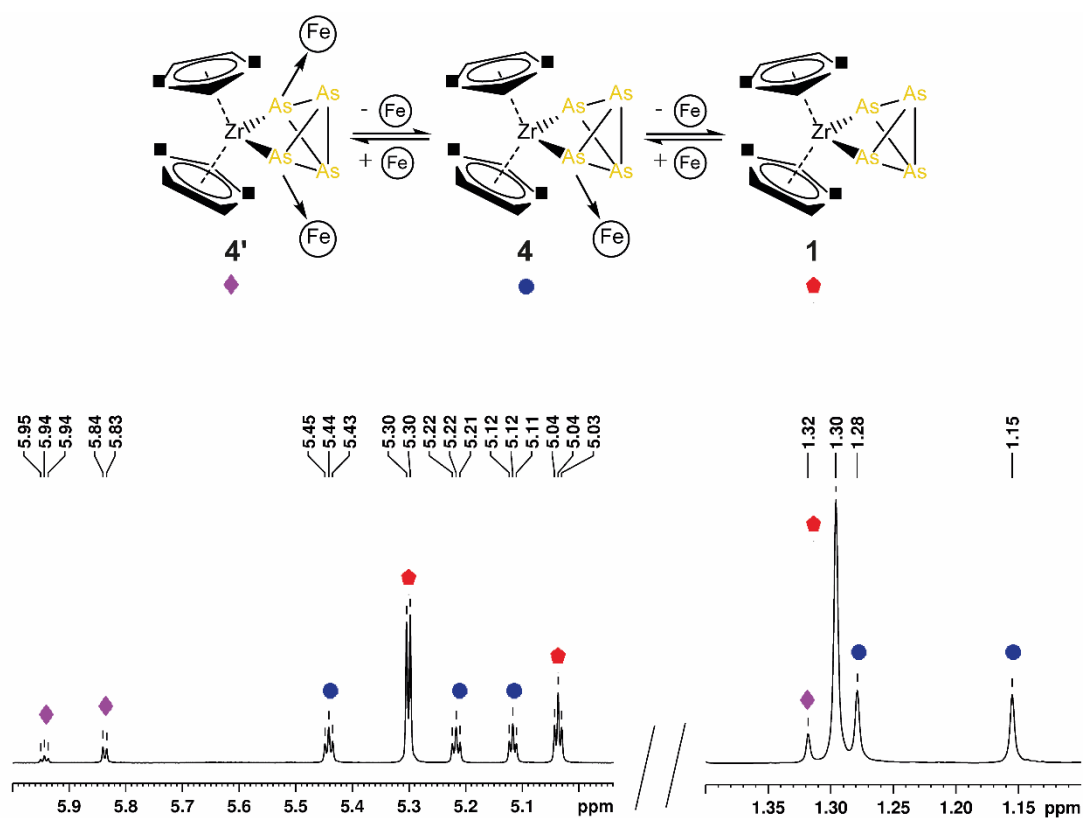
**Figure S9:**  $^1\text{H}$  NMR spectrum of **2** at 293 K in  $\text{C}_6\text{D}_6$  (#). The signal marked with \* is due to silicon grease.



**Figure S10:**  $^1\text{H}$  NMR spectrum of **3** at 293 K in  $\text{C}_6\text{D}_6$  (#). The signal marked with § is due to *n*-pentane. A signal corresponding to the free  $\text{CpMn}(\text{CO})_2$  fragment could not be detected in the  $^1\text{H}$  NMR, probably due to a highly dynamic behavior or a triplet spin state.

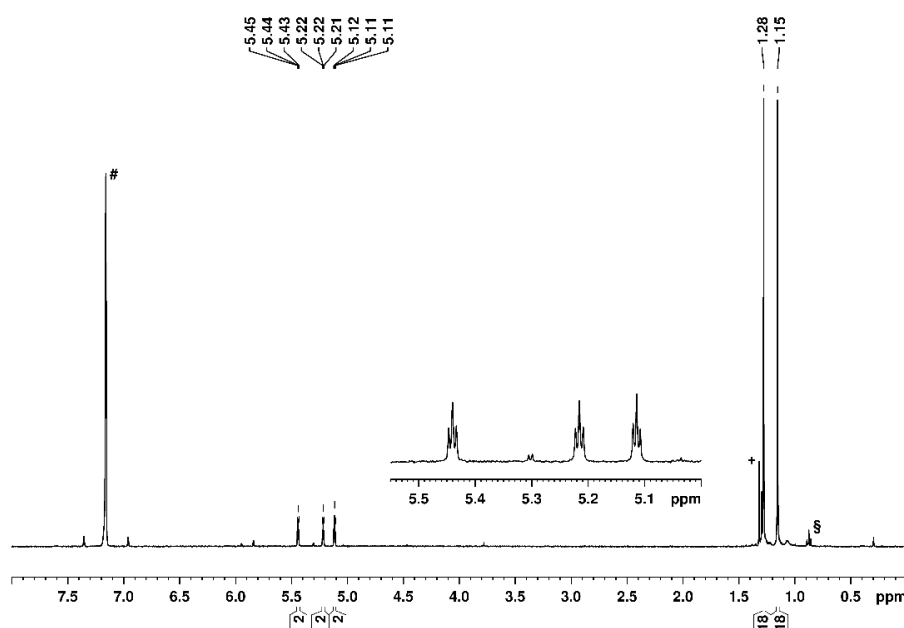


**Figure S11:** Parts of the  $^1\text{H}$  NMR spectrum of **3** at 293 K in  $\text{C}_6\text{D}_6$ .

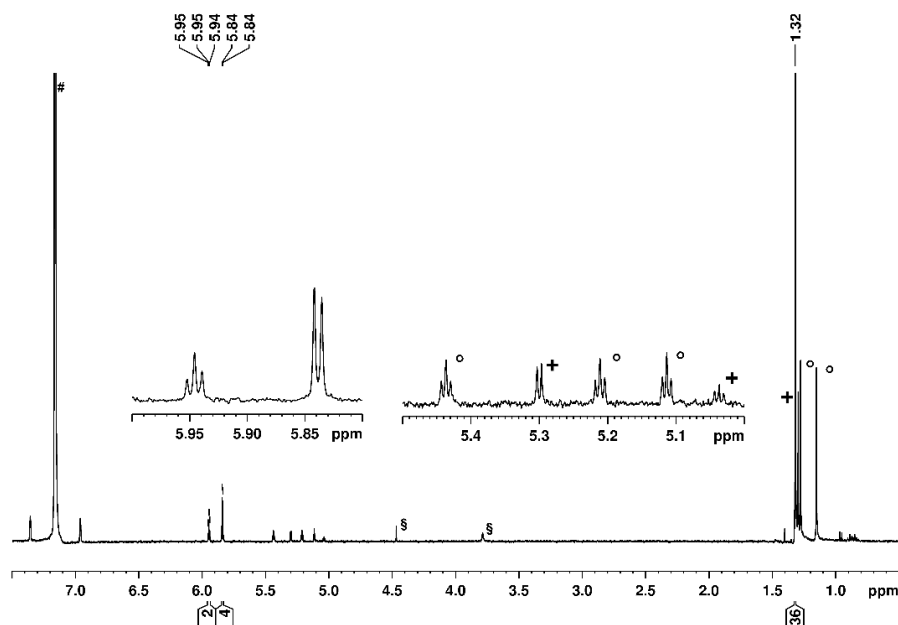


**Figure S12:** Parts of the  $^1\text{H}$  NMR spectrum of the reaction solution of **1** with  $[\text{Fe}_2(\text{CO})_9]$  at 293 K in  $\text{C}_6\text{D}_6$ .

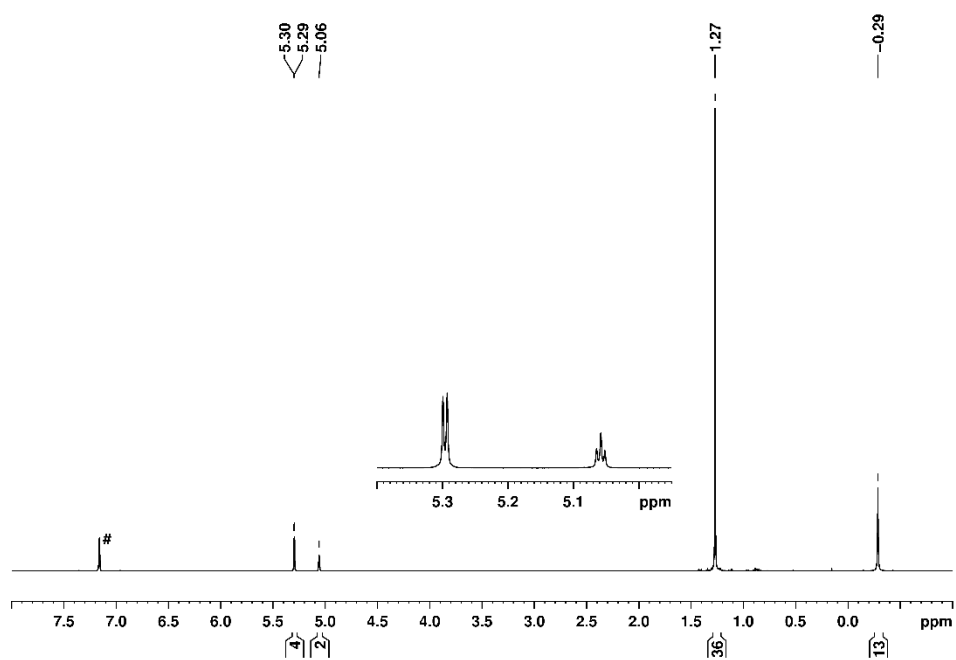




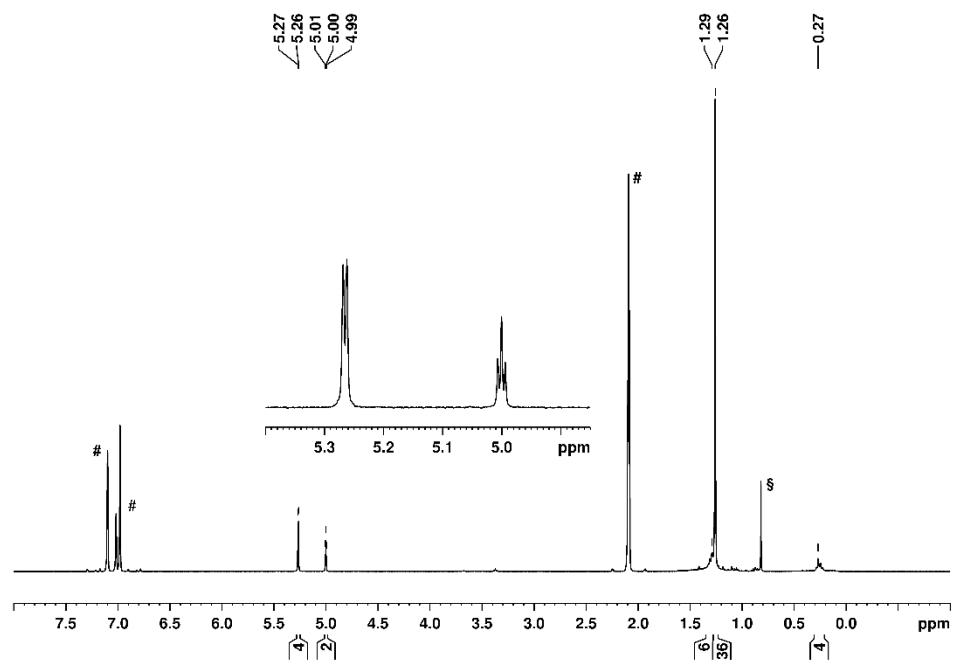
**Figure S13:**  $^1\text{H}$  NMR spectrum of **4** at 293 K in  $\text{C}_6\text{D}_6$  (#). The signal marked with § is due to *n*-pentane, the signal marked with + due to a small amount of starting material **1**.



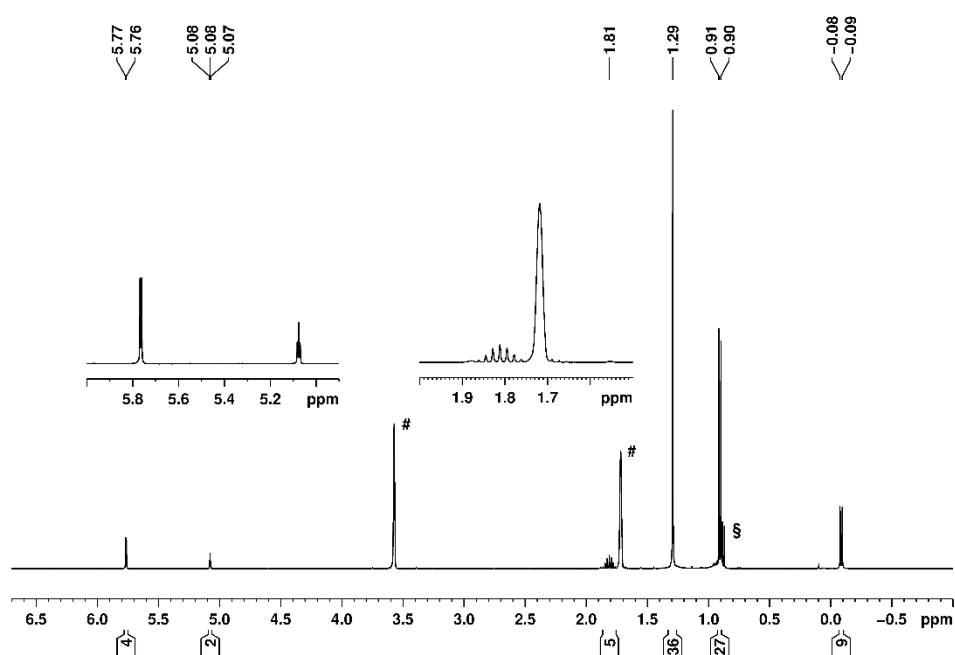
**Figure S14:**  $^1\text{H}$  NMR spectrum of **5** at 293 K in  $\text{C}_6\text{D}_6$  (#). The signal marked with § are due to an unknown impurity, the signal marked with + due to a small amount of starting material **1** and the signals marked with ° due to  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1}\text{-As}_4)(\text{Fe}(\text{CO})_4)]$  (**4**). Especially the signals for **4** were expected to appear in the NMR spectrum due to the co-crystallization of **5** and **4**. The symmetric environment of the  $\text{Cp}''$  ligand in **5** might be an indication of an on the NMR timescale fast dynamic process in solution. Possibly, the  $\text{Fe}(\text{CO})_3$  fragment migrates around the  $\text{As}_4$ -cycle.



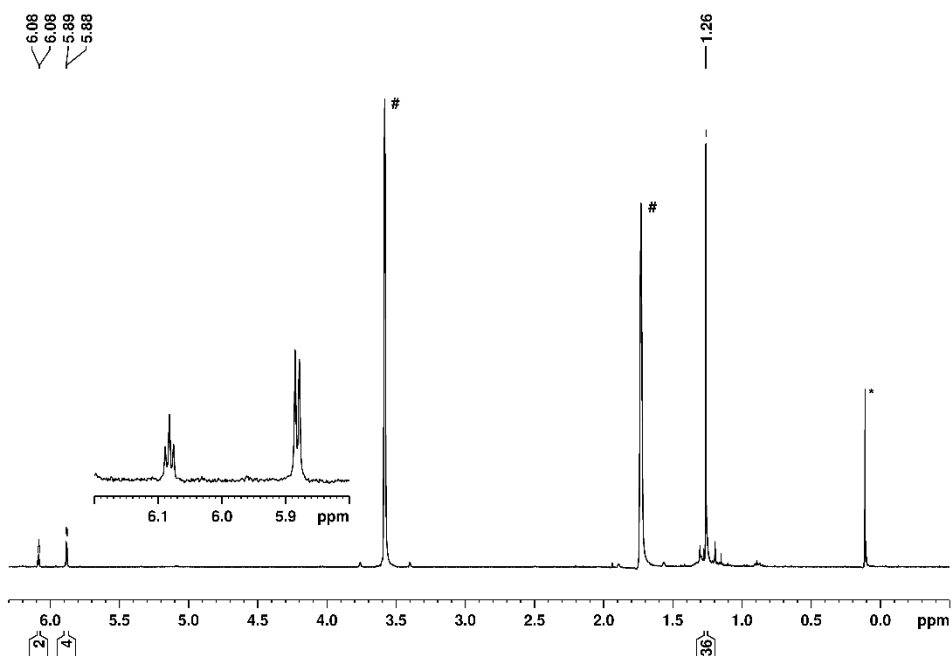
**Figure S15:**  $^1\text{H}$  NMR spectrum of **6a** at 293 K in  $\text{C}_6\text{D}_6$  (#).



**Figure S16:**  $^1\text{H}$  NMR spectrum of **6b** at 293 K in  $\text{tol-d}_8$  (#). The signal marked with § is due to free ethane.



**Figure S17:**  $^1\text{H}$  NMR spectrum of **6c** at 293 K in  $\text{thf-d}_8$  (#). The signal marked with § is due to an unknown impurity.



**Figure S18:**  $^1\text{H}$  NMR spectrum of **7** at 293 K in  $\text{thf-d}_8$  (#). The signal marked with \* is due to silicon grease.

### 3. Computational Details

The geometry of the molecules has been optimized using Gaussian 09 program package.<sup>[5]</sup> Density functional theory (DFT) in form of Becke's three-parameter hybrid functional B3LYP<sup>[6]</sup> with def2-SVP all electron basis set<sup>[7]</sup> or def2-TZVP basis set for all atoms<sup>[8]</sup> was employed. The figures for the supporting information concerning the DFT calculations were created with Chemcraft.<sup>[9]</sup> The reaction energies have been calculated as single point calculations at the B3LYP/def2-TZVP level using the B3LYP/def2SVP optimised geometries. The dispersion effects have been included in the single point calculations via the D3(BJ) model.<sup>[10]</sup> For the calculation of relative energies and reaction energies the SCF energies have been used without corrections for the zero point vibration energies.

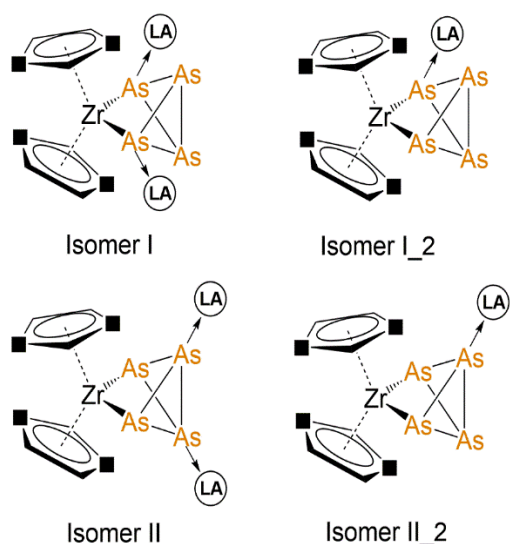
Despite several attempts, the geometry optimization of the isomer of **7** in which the B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> group is bonded to the bridgehead arsenic atoms did not reach convergence, indicating that this isomer is not a stable entity.

**Table S4:** Total and relative energies calculated at the B3LYP/def2-SVP level for the Isomers I, II, I\_2 and II\_2. Labeling according to figure S19.

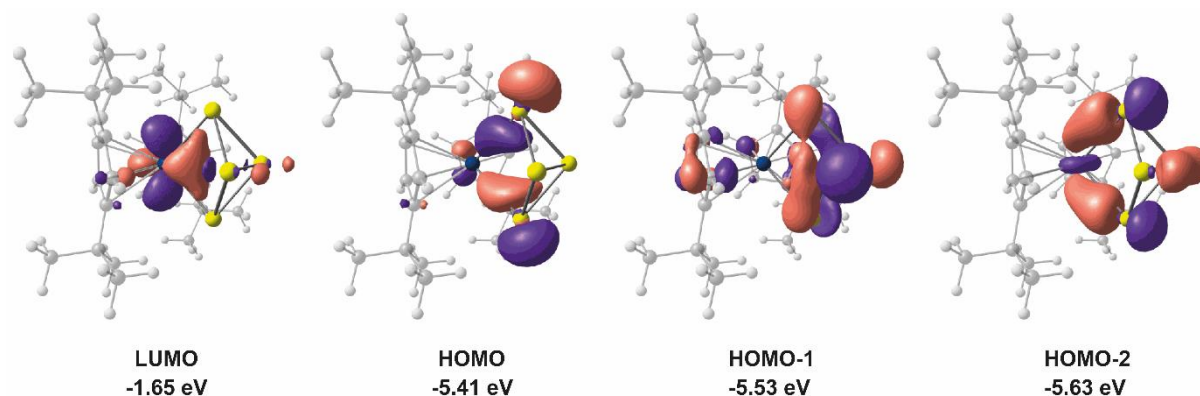
Compound	Total energy [Ha]		$\Delta E$ (Isomer I – II) [kJ·mol <sup>-1</sup> ]
	Isomer I	Isomer II	
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1:1</sup> -As <sub>4</sub> )(W(CO) <sub>5</sub> ) <sub>2</sub> ]	-11272.0985236	-11272.0856656	-33.76
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1:1</sup> -As <sub>4</sub> )(CpMn(CO) <sub>2</sub> ) <sub>2</sub> ]	-13146.7853601	-13146.7796608	-14.96
[Cp <sup>''</sup> <sub>2</sub> Zr(μ,η <sup>1:1:1:1</sup> -As <sub>4</sub> )(Fe(CO) <sub>4</sub> ) <sub>2</sub> ]	-13438.4133113	-13438.4001335	-34.60
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1:1</sup> -As <sub>4</sub> ){AlMe <sub>3</sub> } <sub>2</sub> ]	-10729.2667023	-10729.2540650	-33.18
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1:1</sup> -As <sub>4</sub> ){AlEt <sub>3</sub> } <sub>2</sub> ]	-10964.9386234	-10964.9386234	0.00
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1:1</sup> -As <sub>4</sub> ){Al <sup>i</sup> Bu <sub>3</sub> } <sub>2</sub> ]	-11436.35712	-11436.35027	-17.98
Compound	Total energy [Ha]		$\Delta E$ (Isomer I_2 – II_2) [kJ·mol <sup>-1</sup> ]
	Isomer I_2	Isomer II_2	
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> )(W(CO) <sub>5</sub> )]	-10638.6304544	-10638.6231044	-19.30
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> )(CpMn(CO) <sub>2</sub> )]	-11575.9729414	-11575.9702229	-7.14
[Cp <sup>''</sup> <sub>2</sub> Zr(μ,η <sup>1:1:1</sup> -As <sub>4</sub> )(Fe(CO) <sub>4</sub> )]	-11721.7858591	-11721.7789285	-18.20
[Cp <sup>''</sup> <sub>2</sub> Zr(μ,η <sup>3:1:1</sup> -As <sub>4</sub> )(Fe(CO) <sub>3</sub> )]	-11608.5858271	n.a.	n.a.
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> ){AlMe <sub>3</sub> }]	-10367.2130152	-10367.2066613	-16.68
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> ){AlEt <sub>3</sub> }]	-10485.0492434	-10485.0442703	-13.06
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> ){Al <sup>i</sup> Bu <sub>3</sub> }]	-10720.75877	-10720.75552	-8.53

**Table S5:** Reaction energies (kJ·mol<sup>-1</sup>) for selected transformations at the B3LYP-D3(BJ)/def2TZVP level of theory.

Transformation	Reaction energy [kJ·mol <sup>-1</sup> ]
<b>1</b> + [W(CO) <sub>5</sub> (thf)] = [Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> )(W(CO) <sub>5</sub> ) (I_2) + thf	-57.87
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> )(W(CO) <sub>5</sub> ) (I_2) + [W(CO) <sub>5</sub> (thf)] = <b>2</b> + thf	-58.52
<b>1</b> + [CpMn(CO) <sub>2</sub> (thf)] = [Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> )(CpMn(CO) <sub>2</sub> ) (I_2) + thf	-61.32
[Cp <sup>''</sup> <sub>2</sub> Zr(μ <sub>3</sub> ,η <sup>1:1:1</sup> -As <sub>4</sub> )(CpMn(CO) <sub>2</sub> ) (I_2) + [CpMn(CO) <sub>2</sub> (thf)] = <b>3</b> + thf	-68.44
<b>1</b> + Fe <sub>2</sub> (CO) <sub>9</sub> = <b>4</b> + Fe(CO) <sub>5</sub>	-104.79
<b>4</b> + Fe <sub>2</sub> (CO) <sub>9</sub> = [Cp <sup>''</sup> <sub>2</sub> Zr(μ,η <sup>1:1:1:1</sup> -As <sub>4</sub> )(Fe(CO) <sub>4</sub> ) <sub>2</sub> ] ( <b>I</b> ) + Fe(CO) <sub>5</sub>	-99.52



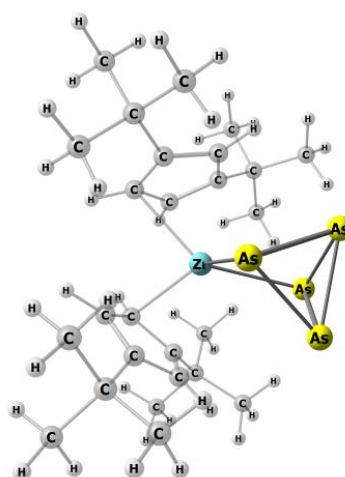
**Figure S19:** Labeling scheme of different isomers.



**Figure S20:** Selected molecular orbitals of **1** at the B3LYP/def2-TZVP level.

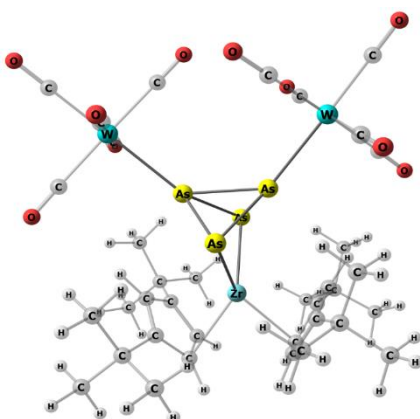
**Table S6:** Cartesian coordinates of the optimized geometry of  $[\text{Cp}''_2\text{Zr}(\eta^{1:1}\text{-As}_4)]$  (**1**) at the B3LYP/def2-TZVP level of theory.

Zr	0.000172299	-0.000051182	-0.534015379
As	-0.202191999	1.812317119	1.474037605
As	0.201814891	-1.811817190	1.474666876
As	-1.207864073	-0.137994761	2.670128421
As	1.207571264	0.138940746	2.670096242
C	-3.459146723	-3.192126687	-2.463524235
H	-4.354209150	-2.631496995	-2.188345006
H	-3.719919244	-4.252653537	-2.502186189
H	-3.160838178	-2.878796176	-3.465349378
C	1.095432641	3.767436752	-1.888609122
H	0.726555796	3.438175688	-2.861941299
H	1.358015017	4.823776598	-1.980089369
H	0.281208500	3.685550986	-1.170108758
C	3.459511178	3.191483769	-2.463895484
H	4.354564302	2.630960055	-2.188485524
H	3.720246434	4.252011656	-2.502762003
H	3.161336848	2.877923515	-3.465678765
C	-3.384728177	2.021343212	-0.798817511
C	2.321121362	2.958194481	-1.440675313
C	-2.650786125	3.350776604	-1.023534349
H	-2.245443522	3.425189519	-2.033718615
H	-1.831399341	3.479180855	-0.316945108
H	-3.342710995	4.184630226	-0.886428361
C	-2.516744152	0.804878606	-1.123052439
C	-2.320858795	-2.958629809	-1.440189195

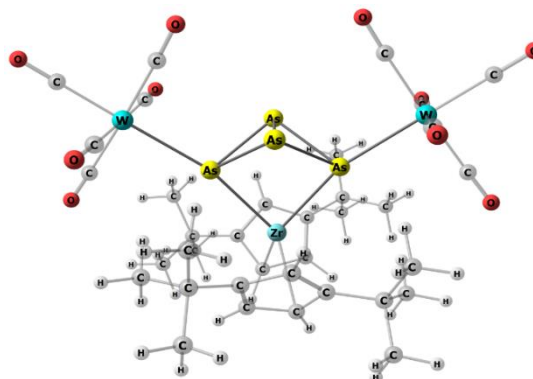


C	-4.584893727	1.962731784	-1.776635147
H	-5.266652520	2.795031021	-1.585068538
H	-5.142233016	1.032082620	-1.656914928
H	-4.253474799	2.025773341	-2.814425510
C	2.650557023	-3.351128554	-1.022151276
H	1.831079665	-3.479023715	-0.315543280
H	3.342273842	-4.185087059	-0.884605599
H	2.245231947	-3.425975564	-2.032306939
C	2.794290311	3.474929900	-0.074666115
H	2.038213547	3.335417869	0.698416706
H	3.009943820	4.543535842	-0.139405423
H	3.709206749	2.976416350	0.249383980
C	1.719141685	-0.656767461	-2.288374926
H	1.445322828	-1.446904084	-2.968189247
C	2.050386994	1.455100881	-1.429236660
C	-3.938944606	1.986590232	0.632603916
H	-4.595054343	2.844856589	0.792350557
H	-3.145678789	2.031256766	1.377426429
H	-4.529874030	1.087440043	0.815188747
C	-1.718778982	0.656155071	-2.288516619
H	-1.444822692	1.446220477	-2.968364987
C	-1.448206183	-0.719971122	-2.482104722
H	-0.931079787	-1.135671676	-3.330874152
C	1.448610400	0.719319329	-2.482240472
H	0.931509076	1.134849525	-3.331109784
C	3.384752482	-2.021744307	-0.798003758
C	-2.794264799	-3.475085652	-0.074155013
H	-2.038430018	-3.335211241	0.699095857
H	-3.009673294	-4.543756069	-0.138659470
H	-3.709357633	-2.976676975	0.249533271
C	-2.050146393	-1.455544109	-1.429048056
C	2.516984615	-0.805282993	-1.122807477
C	2.667471332	0.496330853	-0.584194469
H	3.229520506	0.734534032	0.302678558
C	-2.667289718	-0.496642001	-0.584229130
H	-3.229372071	-0.734658431	0.302676532
C	-1.095162078	-3.767990970	-1.887791601
H	-0.726156288	-3.438957383	-2.861146951
H	-1.357760313	-4.824347310	-1.979069015
H	-0.281028602	-3.685968533	-1.169214740
C	4.584968341	-1.963741538	-1.775802307
H	5.266466498	-2.796189517	-1.584010125
H	5.142574785	-1.033234211	-1.656360186

**Table S7:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu_3\eta^{1:1:1}\text{-As}_4)(\text{W}(\text{CO})_5)_2]$  at the B3LYP/def2-SVP level of theory.



C	-3.623021232	-2.093698411	-1.162577195
C	-2.775015675	-2.575784066	-0.120563953
H	-1.906638381	-3.211442662	-0.275359669
C	-3.314914039	-2.230438204	1.153984018
C	-4.470016707	-1.438065744	0.890076604
H	-5.151172143	-1.040450294	1.640039169
C	-4.664159457	-1.366587545	-0.518250483
H	-5.516579104	-0.902413768	-1.008912780
C	-3.642112185	-2.572673445	-2.617924112
C	-2.254908762	-3.021804820	-3.109651598
H	-1.530696576	-2.191970003	-3.122003738
H	-2.329467551	-3.404332114	-4.139805145
H	-1.836991067	-3.830466816	-2.491968898
C	-4.590820787	-3.799852330	-2.657332656
H	-4.226820247	-4.603730632	-1.998914733



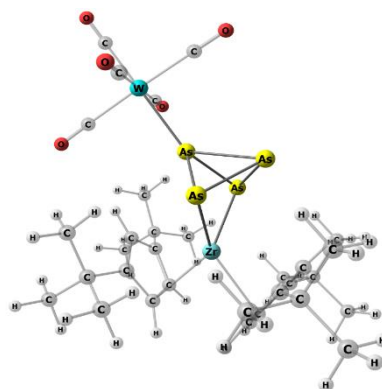
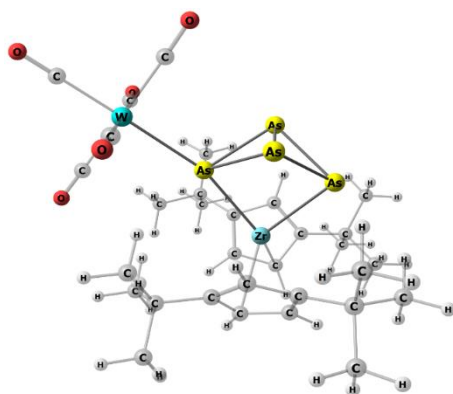
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C	-0.944805782	2.493170909	-2.463610401
C	-0.860874624	3.667916948	-1.656790397
H	-1.700282570	4.294379523	-1.360381963
C	0.511724815	3.973431559	-1.440543543
H	0.884820006	4.866708722	-0.944524688
C	2.802141285	3.100216087	-2.378513889
C	3.383120298	1.780124611	-2.908895757
H	3.279670252	0.967554143	-2.176680749
H	4.456267406	1.897323285	-3.123338984
H	2.893540674	1.462586262	-3.841951412
C	2.928910802	4.171371520	-3.493266246
H	2.357607435	3.882792910	-4.389344027

H	-4.653819005	-4.201453707	-3.681893281
H	-5.608127879	-3.530773250	-2.332964026
C	-4.196055618	-1.493178560	-3.564856186
H	-5.216639222	-1.186645193	-3.286343781
H	-4.243073783	-1.879557048	-4.595215154
H	-3.560435921	-0.596802148	-3.570295588
C	-3.005830345	-2.924044789	2.487331184
C	-3.252257791	-2.010906466	3.701228237
H	-3.114764096	-2.580828453	4.633576134
H	-4.275828807	-1.606188436	3.714373450
H	-2.547541749	-1.166000459	3.723845506
C	-3.985544447	-4.125123826	2.572606891
H	-3.845206963	-4.812678423	1.724095414
H	-5.034221616	-3.789392019	2.565967129
H	-3.813499483	-4.691637700	3.502332031
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H	-1.356138517	-4.167406739	1.726109716
H	-1.418778350	-4.023864764	3.490418410
H	-0.822272345	-2.665688788	2.522819159
C	-3.493904058	2.341903327	1.159098501
C	-2.612051678	2.770320767	0.121485476
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C	-3.495401487	2.829308150	2.612164965
C	-4.342938484	4.129179128	2.629488497
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H	-5.184825853	1.575008873	3.262220252
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H	-1.434692832	2.281789554	3.162246832
H	-2.146704720	3.571323864	4.148197150
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C	-2.815619313	3.144719423	-2.485917989
C	-3.740045177	4.388638025	-2.576057973
H	-3.579578532	5.064582049	-1.721822036
H	-4.802609921	4.100211389	-2.584083047
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H	-2.424950055	1.373336180	-3.729301757
C	-1.357573577	3.628646847	-2.533622683
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C	1.458600430	4.314273741	1.021842437
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C	3.830202508	1.547420016	-0.980438646
C	3.205841247	2.084358861	1.874440163
C	2.817960711	-2.561343004	-2.008377433
C	3.820219055	-1.794371295	0.681876975
C	2.006079671	-3.714310594	1.909824425
C	3.810902561	-4.577038609	-0.176162591
C	0.961662951	-4.466487094	-0.721749247
As	-0.629195078	0.082227542	1.825429385
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As	0.510559573	-1.209802571	0.025114809
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O	0.766651752	5.072670661	1.543858675
O	1.935570221	4.311126814	-2.778471134
O	4.459322394	0.785440555	-1.563241802
O	3.508948842	1.626764641	2.881260893
O	3.052510800	-2.257599650	-3.089038773
O	4.601545950	-1.066614320	1.100731028
O	1.804657797	-4.045832129	2.991581221
O	4.615871355	-5.398954802	-0.255196761
O	0.146352410	-5.198594553	-1.078924205
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W	2.400390923	-3.141603135	-0.046843326
Zr	-2.699987205	0.101061743	-0.002280301

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C	3.608874012	3.567463246	-1.153631824
H	3.245232000	4.533836113	-0.769091825
H	4.668416957	3.699062347	-1.421876566
H	3.565111868	2.833167286	-0.337918719
C	-2.155100747	2.089220894	-3.313173216
C	-3.480165675	2.162060333	-2.535270525
H	-4.324908214	1.947538036	-3.207982923
H	-3.648776226	3.161795507	-2.107122971
H	-3.516424842	1.428944877	-1.717269466
C	-2.217438097	3.123698306	-4.469839125
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H	-3.045823180	2.874679548	-5.152637297
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H	-1.106961143	0.650057896	-4.600827523
H	-2.867411827	0.438983978	-4.541624363
H	-1.873696050	-0.088676940	-3.174122326
C	-1.308379858	2.975366928	2.067417336
C	-0.393111386	2.043561031	2.645735668
H	-0.682108098	1.170511208	3.224727028
C	0.944659454	2.492544643	2.463902930
C	0.860847096	3.667484107	1.657350631
H	1.700328571	4.293904063	1.361059829
C	-0.511713078	3.973177760	1.441150969
H	-0.884725463	4.866588736	0.945311585
C	-2.802219910	3.100115226	2.378979851
C	-2.928859006	4.171145451	3.493861914
H	-2.357529418	3.882420988	4.389877400
H	-3.984722910	4.289752096	3.786655903
H	-2.557002544	5.150999112	3.156274881
C	-3.608912002	3.567616105	1.154170961
H	-3.245113227	4.533962597	0.769719546
H	-4.668430176	3.699368275	1.422449607
H	-3.565273670	2.833398647	0.338383209
C	-3.383332488	1.780025152	2.909200558
H	-3.279846013	0.967520149	2.176928854
H	-4.456497895	1.897253396	3.123547062
H	-2.893854952	1.462377983	3.842274072
C	2.154929834	2.088243917	3.313320438
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H	1.283465214	3.124840043	5.053991159
H	2.382893921	4.142667623	4.091388210
H	3.045781576	2.873104055	5.152982929
C	3.479951601	2.161405984	2.535362232
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H	3.648603857	3.161350479	2.107715618
H	3.516079987	1.428707546	1.716979493
C	1.984141279	0.692147876	3.936463485
H	1.874037380	-0.089648729	3.173322570
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C	-5.737151399	-2.803463466	0.148042064
C	-5.256058280	0.014471102	0.291969314
C	-3.830681503	-1.838860507	2.089719797
C	-2.953696204	-3.400038248	-0.251519127
C	-4.353752935	-1.522113585	-2.020257081
C	4.353954536	-1.522065240	2.020114023
C	2.953803564	-3.399914908	0.251232506
C	3.830892264	-1.838574175	-2.089879609
C	5.737307560	-2.803143774	-0.148212321
C	5.255889780	0.014856572	-0.291812574
As	-1.792445392	-0.116436301	-0.039011522
As	-0.028064161	-1.348124398	1.232826211
As	0.028064962	-1.347956770	-1.233197116
As	1.792373074	-0.116355745	0.038838149
O	-6.688136733	-3.454075966	0.218673975
O	-5.936125379	0.933779490	0.431041303
O	-3.703480506	-1.936090424	3.228254957
O	-2.370807327	-4.375767889	-0.412726850
O	-4.544298090	-1.460619675	-3.153175987
O	4.544663582	-1.460624491	3.153015604
O	2.370859710	-4.375618994	0.412387333
O	3.703962306	-1.935936444	-3.228428887
O	6.688389733	-3.453603400	-0.218924955
O	5.935760882	0.934317245	-0.430844186
W	-4.079255832	-1.667413312	0.032587094
W	4.079336182	-1.667231863	-0.032706568
Zr	-0.000063389	1.979182804	0.000088225



**Table S8:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1}\text{-As}_4)(\text{W}(\text{CO})_5)]$  at the B3LYP/def2-SVP level of theory.

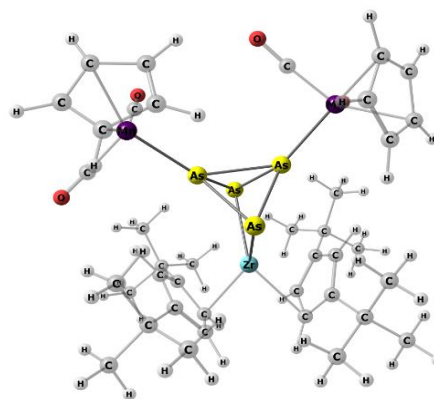
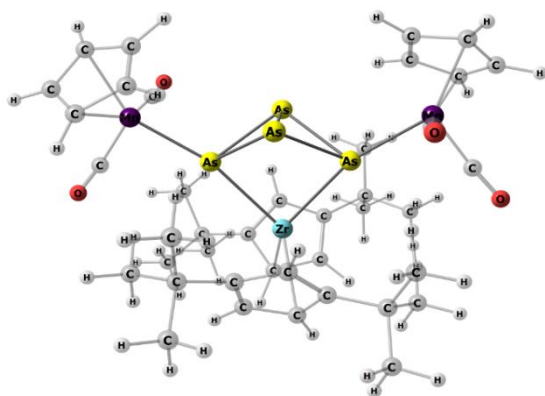


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As	-2.140949484	-0.112005020	-2.161842566	C	-3.930193205	-1.385397394	0.691406981
As	0.003141304	1.152061242	-2.273771698	C	-4.395707780	-0.059244456	0.933807986
As	0.046238818	-1.296845434	-2.123553142	H	-4.701569261	0.340577431	1.898707792
O	3.744636081	0.085372106	-3.368415854	C	-4.516572536	0.618476058	-0.310909062
O	3.424871166	-3.268774895	-0.290225068	H	-4.929431011	1.616356259	-0.441067661
O	6.779389963	-0.274698031	-0.071152918	C	-4.415642077	-0.083454667	-2.844409434
O	3.935211890	3.159097486	-0.017951725	C	-3.636701613	-1.081052667	-3.720248990
O	3.573949118	-0.168179287	3.077833080	H	-2.547737566	-0.950209020	-3.627661434
C	-1.556826946	-2.593791163	0.900638564	H	-3.898889746	-0.935069217	-4.780014433
H	-0.812149168	-3.196930897	0.387147556	H	-3.876476058	-2.124855076	-3.465440143
C	-2.897811012	-2.401243634	0.459473293	C	-5.930842867	-0.368645333	-3.013931800
C	-3.514358034	-1.562261565	1.435218950	H	-6.182841730	-1.385508066	-2.674584972
H	-4.554651247	-1.243223861	1.429987255	H	-6.222192355	-0.279767477	-4.073588407
C	-2.588931961	-1.328905050	2.489380423	H	-6.539795068	0.341064335	-2.432655003
H	-2.809732867	-0.796003547	3.411697373	C	-4.129427498	1.349184726	-3.327543701
C	-1.365375285	-1.981555031	2.175872431	H	-4.677750723	2.098903235	-2.735476059
C	-0.230386334	-2.262478267	3.164127475	H	-4.446411935	1.467121888	-4.376151167
C	1.017744293	-2.806524809	2.451825200	H	-3.058339550	1.586770552	-3.271624620
H	1.399996569	-2.095353683	1.707204505	C	-4.091563553	-2.570548831	1.654344820
H	0.815460278	-3.758949664	1.938663929	C	-3.702837630	-2.218775243	3.100802659
H	1.822515402	-2.989368461	3.180334480	H	-3.949318782	-3.056726200	3.772097920
C	0.143778057	-1.009677446	3.977188855	H	-4.242971149	-1.333647140	3.469743635
H	0.529728842	-0.209650980	3.330637790	H	-2.624082973	-2.025961972	3.194216731
H	0.929058980	-1.250666501	4.710440457	C	-5.601127181	-2.931307128	1.629436463
H	-0.719003881	-0.614783560	4.537072899	H	-5.930370100	-3.188611839	0.610588708
C	-0.748714850	-3.350278643	4.139842007	H	-6.220317904	-2.092091924	1.982388326
H	-1.037316533	-4.264790689	3.598478494	H	-5.797836123	-3.798606122	2.281076329
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C	-3.654757114	-3.282756430	-0.545194502	H	-3.491501704	-4.647189589	1.892300086
C	-4.817859258	-2.546027376	-1.233014407	H	-2.214627658	-3.626432923	1.198468050
H	-5.518989982	-2.111718389	-0.504315945	C	-1.371703356	2.178260465	2.061483561
H	-5.390511514	-3.250783525	-1.856543050	C	-0.414200487	2.404483167	1.029080995
H	-4.460092898	-1.739243986	-1.889563334	H	0.659229914	2.279111303	1.144653787
C	-2.734718198	-3.895409596	-1.615926557	C	-1.050965712	2.934843799	-0.129203999
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H	-3.312005819	-4.586761246	-2.250155380	H	-3.227644048	3.339802801	-0.488978515
H	-1.912818928	-4.475802694	-1.168951850	C	-2.639788372	2.505677383	1.500659687
C	-4.249477685	-4.444802586	0.296036459	H	-3.592338943	2.499021847	2.026561657
H	-4.950653162	-4.070279404	1.057916218	C	-1.071218977	2.015421592	3.55547207
H	-3.456944604	-5.006715962	0.814210065	C	-1.128384296	3.439506812	4.168532569
H	-4.795545785	-5.146699542	-0.355644680	H	-0.398590430	4.107493471	3.685222219
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H	-1.830497506	3.233137739	-0.674757731	H	-2.127073054	3.888537864	4.051634240
C	-3.433372721	2.125260601	0.414948596	C	-2.115676423	1.134459669	4.264151374
C	-3.417143898	1.557621760	1.720789299	H	-3.139387242	1.514047517	4.117708275
H	-4.259431732	1.083630702	2.219820342	H	-1.925815966	1.119011705	5.349272784
C	-2.147183621	1.801757017	2.312535969	H	-2.081414509	0.097085096	3.903164207
H	-1.868761604	1.548754501	3.333943608	C	0.334904636	1.441807652	3.806136817
C	-1.356815674	2.559338724	1.396874645	H	0.450331267	0.433585518	3.379957014
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O	0.610140977	3.918849010	0.522595073	H	1.124028369	2.082064180	3.383598394
H	0.974085006	3.097971084	-0.110017045	C	-0.369207976	3.738688817	-1.245436251
H	1.484399313	4.516294702	0.821889247	C	-0.420236184	5.220612893	-0.785513354
H	-0.033825518	4.564957683	-0.094177731	H	0.082391200	5.351929307	0.185286488
C	-0.676394783	4.626993613	2.547419096	H	-1.458133712	5.572800958	-0.679014327
H	-1.396056691	5.197259348	1.939438465	H	0.085851344	5.866389713	-1.521910911
O	0.150779033	5.302919450	2.819902230	C	-1.098566127	3.628410246	-2.596233279
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C	0.849092254	2.646995401	2.682764946	H	-2.165484967	3.885704290	-2.512665486
H	1.293312425	1.778264606	2.177560056	H	-1.020802593	2.616099551	-3.019759565

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H	1.673032735	3.312262941	2.984881583
C	-4.690946234	2.409154913	-0.413531538
C	-5.437102025	3.563595908	0.305296363
H	-4.798787070	4.457057685	0.388746714
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H	-6.343121263	3.842932390	-0.257354718
C	-4.351314074	2.872343463	-1.841321266
H	-3.749903104	3.794393141	-1.839283521
H	-5.278407309	3.088381636	-2.395536034
H	-3.798197576	2.105835933	-2.404726732
C	-5.624754681	1.187738923	-0.481304316
H	-6.550107092	1.443979914	-1.021556994
H	-5.919189855	0.842359665	0.522504977
H	-5.148486267	0.348089788	-1.005689000
C	3.680267664	0.036743187	-2.222571815
C	3.485997017	-2.121392172	-0.237359207
C	5.627607370	-0.190875349	-0.097470592
C	3.794368730	2.018048179	-0.062854530
C	3.579461055	-0.125712224	1.926560375

C	1.107108074	3.348461427	-1.432968069
H	1.220310947	2.303522805	-1.753650053
H	1.689361759	3.490282549	-0.510009678
H	1.566521230	3.981331873	-2.208357733
C	5.915352156	-0.250347278	-0.005171227
C	3.859048092	-1.491855447	1.633176518
C	3.723507420	1.377047030	1.014895684
C	3.925923793	0.779115125	-1.853699907
C	4.016604082	-2.098192005	-1.247515536
As	-0.430434139	-1.331005529	1.437237243
As	1.205778364	-0.505365635	-0.220635020
As	-0.275033536	-2.327714339	-0.874502023
As	-0.468298183	-0.086850649	-2.001431939
O	7.066410200	-0.193154794	0.054527045
O	3.843503346	-2.117529417	2.595633573
O	3.601844818	2.340199424	1.636108319
O	3.942637136	1.407645228	-2.815549202
O	4.072780221	-3.058742111	-1.872487420
W	3.904547085	-0.351473392	-0.109655377
Zr	-2.053828948	0.458525580	0.159742468

**Table S9:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu_3, \eta^{1:1:1:1}\text{As}_4)(\text{CpMn}(\text{CO})_2)_2]$  at the B3LYP/def2- SVP level of theory.



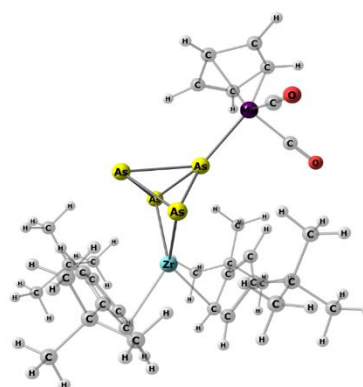
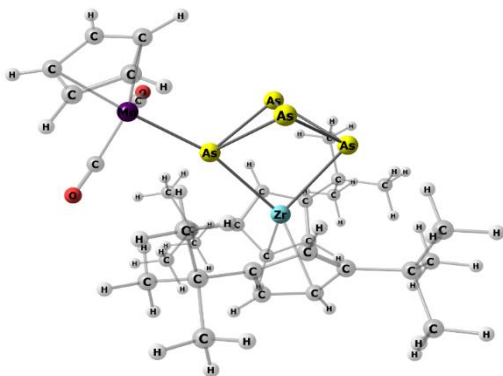
Zr	0.008041933	1.510709488	-0.012297642
As	-1.826715503	-0.527014655	-0.001777666
As	1.823167126	-0.541723280	0.019012667
As	0.002583081	-1.735545915	-1.217404557
As	-0.014925864	-1.718154653	1.253047433
Mn	3.868500494	-1.843580541	-0.109693459
Mn	-3.898986210	-1.792437401	0.141343503
O	5.654295525	0.487139023	-0.253336333
O	-5.648723553	0.555805147	0.379632828
O	3.640339796	-2.178941680	-3.021805497
C	0.354874212	1.588356951	-2.680664933
H	0.654957003	0.723000201	-3.266314406
C	-0.311478012	1.640597874	2.654898292
H	-0.596879736	0.784477141	3.261331297
C	3.323580603	-3.868956459	0.531758941
H	2.455724580	-4.425839926	0.183992836
C	-1.230590178	2.574002665	2.085294907
C	-0.988763472	2.006388515	-2.470006111
C	1.026261808	2.067373727	2.421174576
C	2.257581891	1.678134073	3.248278976
C	1.259469613	2.541135953	-2.118813507
C	0.452564869	3.520710669	-1.478710288
H	0.816011395	4.421862328	-0.990362545
C	-0.915283015	3.184476425	-1.667013699
H	-1.762105999	3.789441413	-1.349203787
C	3.572860643	1.945681910	2.498076514
H	3.656235371	1.331208157	1.592092779
H	4.432070364	1.703537338	3.143225434
H	3.674330026	3.002212937	2.207104774
C	2.228352939	0.214512649	3.720145271
H	1.300826636	-0.028499944	4.261044828
C	3.066151307	0.030798592	4.411685922
H	2.331613883	-0.483272418	2.878819344
C	-0.440496022	3.546190591	1.413544972
H	-0.818289567	4.432884202	0.909731834
C	0.932585709	3.228120509	1.596395736

Zr	2.053574546	0.271579083	0.042035706
As	-0.056326160	0.027712440	1.788066011
As	0.088118922	0.014304330	-1.863413326
As	-1.333656723	1.070432508	-0.092192061
As	-0.991668745	-1.341799364	-0.088356969
Mn	-3.261779616	2.479570350	-0.063944834
Mn	-2.361884478	-3.267400368	-0.127600301
O	-2.896733470	3.589825668	-2.767508798
O	-2.963902446	-3.011824976	-3.001518439
O	-5.058984328	0.320979313	-0.933564596
C	1.725635775	2.916535997	0.168278272
H	0.755703636	3.389204101	0.305234080
C	2.394995961	-2.389490284	-0.068882444
H	1.597936128	-3.106746494	-0.244187918
C	-4.832208550	3.083519333	1.278081645
H	-5.842997274	2.679444899	1.240542631
C	2.871778968	-2.002708923	1.218103261
C	2.617580226	2.561616657	1.226186693
C	3.212941488	-1.818488961	-1.089557678
C	3.322087958	-2.301564749	-2.539496011
C	2.343418679	2.678563067	-1.096412127
C	3.602419246	2.076735603	-0.810635975
H	4.352357574	1.796345920	-1.547414365
C	3.774880947	2.019244252	0.599515664
H	4.678438209	1.686317381	1.105704760
C	3.755347994	-1.170128571	-3.487864987
H	3.007805208	-0.365662553	-3.519543061
H	3.879934702	-1.557682748	-4.511476532
H	4.718958534	-0.728945751	-3.187068732
C	2.010706496	-2.924732683	-3.049930522
H	1.685033205	-3.772517303	-2.428715104
H	2.151406561	-3.304713661	-0.474253239
H	1.190613191	-2.191526309	-3.081807471
C	3.949036350	-1.099406635	0.984723394
H	4.568377168	-0.638241172	1.751698124
C	4.166192277	-1.000149858	-0.418312852

H	1.770161018	3.832947122	1.256042503
C	4.621947755	-3.859720364	-0.067150362
H	4.915630783	-4.406274031	-0.962384505
C	3.386268776	-3.038853926	1.687553476
H	2.562517761	-2.844059521	2.371910154
C	4.906693101	-0.398992191	-0.212264826
C	3.708045125	-2.003632581	-1.878878547
C	2.741466817	2.710394121	-2.464143690
C	5.470530576	-3.028481909	0.711571587
H	6.524727169	-2.833136519	0.522160901
C	3.348277199	1.406931892	-3.003573769
H	3.266296186	0.593772281	-2.272360583
H	4.417305292	1.546501359	-3.225485471
H	2.857311860	1.079433649	-3.932477483
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H	5.062312043	-1.866793578	2.600043858
C	-2.710003017	2.738602539	2.442165281
C	-2.208075697	1.588301075	-3.301010124
C	2.214968056	2.590328121	4.504355743
H	2.240253849	3.655445817	4.226512747
H	3.082691652	2.385033739	5.152622787
H	1.300462572	2.415808396	5.092244615
C	-3.295992973	1.444598009	3.026335196
H	-3.200486381	0.607114665	2.324914531
H	-4.366840780	1.573985862	3.245083831
H	-2.797757665	1.158776205	3.965238609
C	-4.909400265	-0.334878178	0.301814369
C	-3.530095628	1.760737504	-2.534818777
H	-3.596117962	1.072378330	-1.681968269
H	-4.382334524	1.547138446	-3.199411236
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H	-2.120077140	-0.587524036	-3.009044123
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H	3.177173049	4.158395332	-0.865640172
H	4.609802449	3.366066164	-1.550210728
H	3.559447000	2.467384202	-0.442447869
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H	-4.592859728	3.358011145	1.531928109
H	-3.550369080	2.439121649	0.434834544
C	-2.780200115	3.840074415	3.532027268
H	-2.181550159	3.565291307	4.414690654
H	-3.823169149	3.982965671	3.859209327
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H	-3.070174848	2.304653165	-5.185229742
H	-1.294316755	2.455309097	-5.110371445
C	-4.640742522	-2.402015968	-1.836046332
H	-4.874982313	-1.727770063	-2.657401978
C	-4.843282119	-3.722234368	0.047491722
H	-5.259798696	-4.227715059	0.917554334
O	-3.616874246	-2.198585988	3.040163788
C	-3.704663196	-1.998896011	1.902704488
C	-5.538618860	-2.820190473	-0.800067232
H	-6.578680653	-2.516079098	-0.692435892
C	-3.399312699	-3.052190325	-1.610245432
H	-2.508243522	-2.950672031	-2.226972612
C	-3.509490894	-3.870002823	-0.453133515
H	-2.731055349	-4.507308156	-0.038054580

H	4.978870284	-0.450431911	-0.888074779
C	-3.754211321	2.570301668	2.063785006
H	-3.794118657	1.719372417	2.740801223
C	-4.366929327	4.218550662	0.560865198
H	-4.958261095	4.837231051	-0.112016036
C	-3.010239603	3.115363389	-1.719440712
C	-4.311364012	1.147960002	-0.622393467
C	1.972831142	3.339919628	-2.431143376
C	-2.621881506	3.402568546	1.822752463
H	-1.637451588	3.273961076	2.267212128
C	0.473818594	3.659184470	-2.540296508
H	-0.141051015	2.749608441	-2.553053844
H	0.269725788	4.203444498	-3.475372535
H	0.123956944	4.294655161	-1.712657750
C	-2.990402711	4.420857468	0.907093309
H	-2.348098400	5.219201138	0.539116722
C	2.597454827	-2.732378801	2.539412375
C	2.551043929	3.038336513	2.681517469
C	4.415666647	-3.401951933	-2.549482221
H	5.387992313	-3.004566035	-2.218631132
H	4.540705273	-3.808256929	-3.566813390
H	4.145393135	-4.234822921	-1.881875384
C	1.270252589	-3.509823620	2.505189836
H	0.410395315	-2.849685538	2.323647278
H	1.109829501	-4.016540549	3.470380182
H	1.269646411	-4.283607983	1.723631140
C	-2.692051599	-3.085549278	-1.882120626
C	3.156257138	2.012660562	3.656128942
H	2.564878157	1.087318703	3.681418773
H	3.180417207	2.426432169	4.677064788
H	4.191367192	1.750684258	3.386510012
C	1.115123374	3.364363637	3.123976770
H	0.662080337	4.145663714	2.494659632
H	1.116073453	3.739289957	4.159723281
H	0.468876760	2.474203302	3.092978361
C	2.399388280	2.498531236	-3.647319438
H	3.473120812	2.256627657	-3.628409553
H	2.206166971	3.057500524	-4.576573922
H	1.836049798	1.555700942	-3.704889080
C	2.609731390	-1.788814363	3.754759565
H	3.544074861	-1.210304697	3.817361487
H	2.521405018	-2.371683687	4.685597766
H	1.769187269	-1.079637774	3.724387764
C	3.750351089	-3.757788782	2.707490208
H	3.793367845	-4.448071933	1.850818675
H	3.598704479	-4.356364774	3.620970517
H	4.727021565	-3.255432056	2.787138676
C	2.756947468	4.679276161	-2.465798464
H	2.483689275	5.320822046	-1.613388718
H	2.530857007	5.230485568	-3.393483092
H	3.844329169	4.510094750	-2.425209765
C	3.387415334	4.342883053	2.752408202
H	4.439093906	4.159216414	2.483350416
H	3.364129958	4.759684168	3.772970475
H	2.992239814	5.105567097	2.063229407
C	-3.372366316	-4.736031654	1.076985294
H	-3.111640754	-5.793457711	1.085645952
C	-4.371773363	-2.724614791	0.534804742
H	-4.988003423	-1.971167128	0.048358226
O	-0.138153426	-5.148286201	-0.537828297
C	-0.999921788	-4.383694954	-0.394980860
C	-4.309087508	-4.117987278	0.205684804
H	-4.890349705	-4.619250538	-0.566707701
C	-2.844758929	-3.733442305	1.951601170
H	-2.118967694	-3.888805152	2.747696455
C	-3.464804035	-2.499268174	1.604719318
Zr	2.053574546	0.271579083	0.042035706

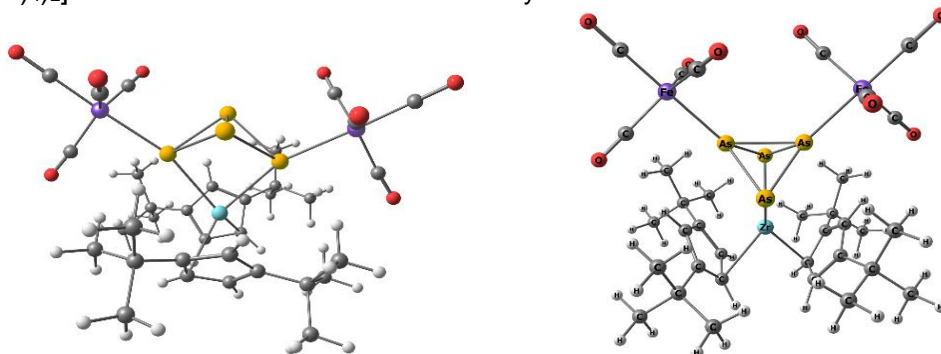
**Table S10:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu_3\eta^{1:1:1}\text{-As}_4)(\text{CpMn}(\text{CO})_2)]$  at the B3LYP/def2- SVP level of theory.



Zr	1.257331367	0.047352463	0.524050588
As	1.695748828	0.022326011	-2.165797944
As	-1.374392899	-0.026658240	-0.210771919
As	-0.440330943	-1.243841300	-2.216569521
As	-0.479528104	1.215161713	-2.220514829
Mn	-3.782290323	-0.185902383	-0.193627852
O	-3.978772380	-0.094136074	2.738323493
O	-3.724166859	-3.121330942	-0.355803974
C	1.150757164	-2.613378506	0.808130279
H	0.429604302	-3.229710919	0.276789534
C	1.461789295	2.740956145	0.354476130
H	1.104916979	3.313734186	-0.497631309
C	-4.312692411	0.419501622	-2.233630847
H	-3.777296477	0.126052509	-3.134492787
C	2.786690659	2.229489167	0.490799194
C	2.481314835	-2.351041155	0.371444837
C	0.712511030	2.489140901	1.537127095
C	-0.543547459	3.243644257	1.987901766
C	0.937688073	-2.049711849	2.103536176
C	2.135503927	-1.358819223	2.434586891
H	2.338663566	-0.848629542	3.373328297
C	3.065694294	-1.519014469	1.372296071
H	4.091804292	-1.156381631	1.373872178
C	-1.358524741	2.451723730	3.023396654
H	-1.745933828	1.513647977	2.604711069
H	-2.223279081	3.045136155	3.359546955
H	-0.764001643	2.209256059	3.917348952
C	-1.458624471	3.630566850	0.813583710
H	-0.923030672	4.206314158	0.042955772
H	-2.284373209	4.262251744	1.178244382
H	-1.901343137	2.744177580	0.339818860
C	2.830942281	1.586208243	1.760605273
H	3.708418433	1.130959416	2.214224229
C	1.564544234	1.726944848	2.390673895
H	1.320346259	1.395873135	3.397882057
C	-5.396573028	-0.282292976	-1.628977713
H	-5.825409433	-1.218719393	-1.983750884
C	-4.081583413	1.594469483	-1.455580035
H	-3.327881655	2.353341657	-1.657758690
C	-3.855749508	-0.143820622	1.585628143
C	-3.705081055	-1.966566604	-0.266380118
C	-0.172135466	-2.420694486	3.091698736
H	-5.828947936	0.445864633	-0.486515843
H	-6.648944967	0.174206913	0.175815205
C	-1.425316742	-2.944253830	2.374328129
H	-1.855134549	-2.183332152	1.710780192
H	-2.198461430	-3.215422922	3.109792719
H	-1.214199166	-3.840992993	1.772456854
C	-5.010551391	1.617392367	-0.385984688
H	-5.092240403	2.391726053	0.375141159
C	4.011575025	2.634652161	-0.337423942
C	3.273086012	-3.159332229	-0.666486495
C	-0.033225328	4.547754739	2.656913500
H	0.619576826	4.327566086	3.515914873
H	-0.883130396	5.149275270	3.019502602
H	0.540901049	5.161656642	1.945454406
C	3.619378122	3.178517720	-1.722952867
H	3.087903069	2.427793690	-2.326452024
H	4.523081993	3.474883396	-2.278805624

Zr	-1.497270412	0.447226805	0.249804540
As	0.107242259	-1.538062654	1.210129037
As	-0.001345078	0.155875288	-2.021659994
As	0.122885607	-2.224934348	-1.222554743
As	1.716973524	-0.565768311	-0.393521290
Mn	4.079102736	-0.470603777	-0.303627708
O	4.343947747	0.876986246	-2.910019169
C	-3.237404527	-1.344063338	-0.763032106
H	-2.938401966	-2.195372030	-1.369223584
C	0.240819554	2.241376536	1.257453157
H	1.316777266	2.090971926	1.289030756
C	-0.657403506	1.900799646	2.311035863
C	-3.426500148	-1.377949812	0.649286303
C	-0.453915994	2.925943483	0.219254126
C	0.175027915	3.849384738	-0.832541739
C	-3.607908137	-0.068695049	-1.282022687
C	-3.966226683	0.725725390	-0.154607525
H	-4.349544590	1.743411648	-0.186887995
C	-3.845889914	-0.066552111	1.020755798
H	-4.125367232	0.250311795	2.023780026
C	-0.660732756	3.931151614	-2.121381980
H	-0.672559190	2.968859101	-2.652937802
H	-0.231819861	4.683508246	-2.802222233
H	-1.702781403	4.224997136	-1.921511538
C	1.617628475	3.447175537	-1.186800787
H	2.274248487	3.443490405	-0.304392876
H	2.039319512	4.168884747	-1.904235118
H	1.667727432	2.453290412	-1.654653034
C	-1.950111271	2.314510446	1.877746690
H	-2.868868647	2.255102912	2.457185469
C	-1.828643650	2.925878171	0.598052319
H	-2.636588908	3.409623638	0.052626400
C	-3.943464695	0.252157799	-2.742282130
C	-3.232965534	-0.700809788	-3.720038769
H	-2.137573195	-0.630862340	-3.640823633
H	-3.509331914	-0.450707089	-4.756630503
H	-3.519967757	-1.750021199	-3.549973780
C	-0.270408399	1.548552207	3.751083799
C	-3.598772526	-2.640815145	1.505794786
C	0.214574512	5.259774063	-0.185348057
H	-0.797610632	5.619542338	0.057112851
H	0.678751791	5.983423294	-0.875673188
H	0.802613135	5.251878690	0.745527732
C	1.114009350	0.880720057	3.835850654
H	1.136886143	-0.083842848	3.306192965
H	1.371822347	0.687785794	4.889593590
H	1.906883486	1.517547918	3.415126330
C	4.202709508	0.363423164	-1.884491197
C	-3.147391726	-2.440621094	2.963496419
H	-2.057895279	-2.308854959	3.036021733
H	-3.415685035	-3.323936014	3.564954597
H	-3.630177720	-1.567893794	3.429091857
C	-2.866962921	-3.857978905	0.912265244
H	-3.214370447	-4.087831504	-0.106807609
H	-3.061278458	-4.748105950	1.531594399
H	-1.778498444	-3.707173787	0.876643614
C	-3.600435593	1.706562507	-3.109323974
H	-4.094130714	2.426403144	-2.437613658
H	-3.937584658	1.930949324	-4.133932627

**Table S11:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1:1}\text{-As}_4)(\text{Fe}(\text{CO})_4)_2]$  at the B3LYP/def2- SVP level of theory.

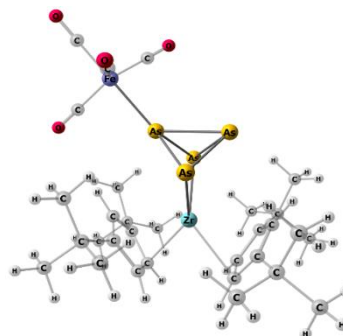
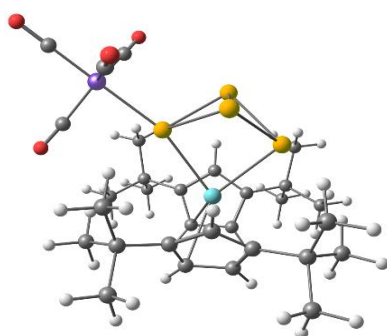


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As	-0.024696323	-1.855646597	1.227965765	As	-1.215999015	1.207001943	-0.015669481
Fe	-3.890859910	-1.933966386	0.011304099	Fe	-2.993824721	2.862855542	-0.064521718
C	0.471323292	1.595876840	-2.643333314	C	2.038481506	-2.674450439	0.232938404
H	0.779736067	0.734744856	-3.211471518	H	1.164538808	-3.273804169	0.425772502
C	-1.932975993	0.194830088	-3.910310910	C	0.782272678	-3.656293167	-2.380492842
H	-1.975558135	-0.543945094	-3.112820433	H	0.056656473	-2.843631819	-2.384366907
H	-1.008550304	0.042823875	-4.469744244	H	0.562618759	-4.306329970	-1.533077805
H	-2.760991864	-0.010020174	-4.590957865	H	0.620807100	-4.240914804	-3.288017547
C	1.360267978	2.530218507	-2.043772739	C	2.907975698	-2.172699315	1.239356120
C	-0.815553376	3.196306743	-1.682623110	C	3.742920150	-1.634689563	-0.841218870
H	-1.658527839	3.808656844	-1.406833126	H	4.419492027	-1.291845005	-1.607047989
C	0.543454880	3.510999642	-1.431445493	C	3.955342539	-1.506908196	0.555088820
H	0.892448540	4.394338613	-0.923660991	H	4.815545209	-1.045342072	1.010031767
C	-0.868391031	2.030487893	-2.494541240	C	2.569422969	-2.403052314	-1.056389213
C	-2.010498651	2.595090759	-4.586102198	C	3.171376367	-4.371779570	-2.393327888
H	-2.820666562	2.361292810	-5.271380449	H	2.974811483	-4.960931160	-3.291756317
H	-1.071385948	2.504052137	-5.134361034	H	3.017524755	-5.014927374	-1.525429759
C	-2.119112027	3.633376951	-4.268569485	H	4.219207350	-4.067556263	-2.407775719
C	-3.434952421	-2.521458671	1.657841501	C	-3.182829138	2.673488919	1.730190144
C	3.474301126	1.374189235	-2.840793751	C	1.546036350	-2.975650911	3.239211609
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C	2.971193424	3.740028868	-3.451588828	C	3.842621128	-3.841709604	2.785839969
H	4.020534869	3.875179065	-3.722506915	H	3.907820739	-4.193677331	3.817778352
H	2.576109658	4.705373003	-3.131160716	H	4.852712809	-3.619345647	2.437661967
H	2.427349313	3.431485427	-4.346022450	H	3.445454034	-4.654491341	2.175670375
C	-3.363758391	-2.777205035	-1.498042836	C	-3.913497383	1.785508624	-1.200386926
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C	2.850936074	2.678791338	-2.329522924	C	2.933171276	-2.590585852	2.707657994
C	-3.394704052	1.802844651	-2.663232395	C	2.490712288	-2.294585758	-3.601924613
H	-3.541892507	2.825441234	-2.312768241	H	3.518709496	-1.931071204	-3.640801075
H	-3.483133317	1.132745532	-1.811203942	H	1.822058981	-1.435016545	-3.653044500
H	-4.212535181	1.572772242	-3.348080477	H	2.323923652	-2.895652726	-4.497824791
C	3.627679855	3.182618859	-1.104316580	C	3.531886723	-1.496864025	3.603334516
H	3.599185962	2.465788865	-0.285813536	H	2.919918016	-0.595921719	3.591904091
H	3.236237882	4.136067730	-0.743410642	H	4.544259375	-1.227959341	3.296308580
H	4.675707649	3.339054079	-1.364909281	H	3.588971899	-1.849739254	4.634863394
C	-4.895663856	-0.4411505298	-0.095981020	C	-1.827903855	4.067178414	-0.727768326
Zr	-0.000011414	1.522229338	0.000137209	Zr	2.032495755	0.000747254	0.000328644
As	1.774374613	-0.609845547	0.040740972	As	-0.049964078	0.014080868	1.829714335
As	0.024908441	-1.855065333	-1.228740592	As	-1.214805302	-1.207962892	0.014367229
Fe	3.891056547	-1.933668887	-0.011592828	Fe	-2.991124578	-2.865461328	0.062615383
C	-0.471590460	1.595157514	2.643487178	C	2.036536743	2.675809006	-0.232156911
H	-0.780055055	0.733834989	3.211310098	H	1.162272421	3.274558691	-0.425400854
C	1.932255370	0.193944456	3.910771278	C	0.778295133	3.657072074	2.380465161
H	1.974565377	-0.544817411	3.113254734	H	0.053075321	2.844050779	2.383984645
H	1.007833136	0.042168505	4.470274786	H	0.558785711	4.306936286	1.532874278
H	2.760272543	-0.011156142	4.591342222	H	0.616032598	4.241688805	3.287865382
C	-1.360474850	2.529712323	2.044141406	C	2.907062269	2.174959912	-1.238088767
C	0.815388225	3.195869331	1.683385432	C	3.741162726	1.637332994	0.842947803
H	1.658391671	3.808304301	1.407862757	H	4.417529457	1.294894977	1.609136826
C	-0.543592794	3.510670970	1.432202561	C	3.954503650	1.509843939	-0.553279976
H	-0.892520530	4.394178135	0.924664243	H	4.815377518	1.049045058	-1.007735387
C	0.868133486	2.029817271	2.494977255	C	2.566960914	2.404740331	1.057473259
C	2.010153881	2.594169297	4.586635820	C	3.166950609	4.373872937	2.394689356
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H	1.070899454	2.503398249	5.134696130	H	3.013263359	5.016890786	1.526665251
H	2.119150519	3.632431120	4.269156417	H	4.214950405	4.070254617	2.409808669
C	3.435107380	-2.521314312	-1.658062401	C	-3.175234953	-2.686518168	-1.733674236
C	-3.474577902	1.373424658	2.840572217	C	1.545678743	2.976900182	-3.238722961
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H	-4.535397122	1.526799609	3.044663568	H	1.634043040	3.339308259	-4.264779592
H	-3.007894766	1.042797142	3.769754649	H	1.084979363	3.771353002	-2.651615028
C	-2.971408370	3.738988723	3.452414773	C	3.841335926	3.844632594	-2.784040581



H	-4.020754658	3.874047150	3.723356599	H	3.906913804	4.196608719	-3.815953627
H	-2.576290562	4.704459066	3.132411728	H	4.851392146	3.623085871	-2.435211924
H	-2.427600296	3.430046139	4.346732426	H	3.443135613	4.657135311	-2.174161145
C	3.364101652	-2.776835029	1.497847332	C	-3.911511513	-1.782181036	1.192109636
C	2.048550040	1.627006221	3.375809625	C	2.224369959	3.144745691	2.350852805
C	-2.851147903	2.678224679	2.329893014	C	2.932781950	2.592800326	-2.706380439
C	3.394430880	1.801714492	2.663899973	C	2.486799207	2.296304949	3.602947317
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H	3.482982956	1.131373179	1.812074380	H	1.818688509	1.436286306	3.653662622
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C	-3.627822643	3.182592617	1.104868877	C	3.532879550	1.499578541	-3.601763648
H	-3.599308631	2.466107387	0.286067180	H	2.921623592	0.598140660	-3.590846457
H	-3.236328715	4.136178757	0.744379925	H	4.545274623	1.231436306	-3.294123433
H	-4.675855576	3.338958308	1.365481708	H	3.590338214	1.852615793	-4.633214446
C	4.895744534	-0.441120916	0.095603043	C	-1.826392636	-4.068542422	0.730290623
C	5.364364972	-2.931299217	-0.052577585	C	-4.305726909	-4.068529928	0.098826245
C	-5.364096256	-2.931698915	0.052258207	C	-4.305056934	4.069764445	-0.093141216
O	5.599359253	0.464962358	0.147933458	O	-1.094590587	-4.849530279	1.147764932
O	6.309090615	-3.573578477	-0.079019688	O	-5.147868436	-4.839174386	0.122956108
O	3.064840546	-3.324679757	2.460130351	O	-4.510903899	-1.124899722	1.910607846
O	3.188598557	-2.898213531	-2.713011786	O	-3.299881384	-2.609310313	-2.868324674
O	-3.064390856	-3.325091494	-2.460269059	O	-4.512581417	1.132078393	-1.922579904
O	-3.188478656	-2.898299385	2.712819960	O	-3.310516603	2.589493059	2.864019240
O	-6.308742575	-3.574095726	0.078674847	O	-5.144597317	4.843411069	-0.111287815
O	-5.599314961	0.464546502	-0.148370061	O	-1.095109705	4.848930768	-1.142172084

**Table S12:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1}\text{-As}_4)(\text{Fe}(\text{CO})_4)]$  at the B3LYP/def2-SVP level of theory.

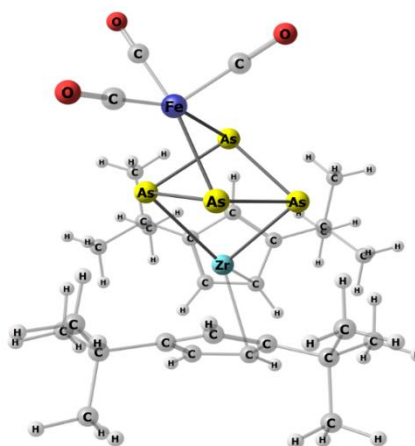


As	-0.454739521	-1.224162621	-2.249529099	As	-1.777766655	-0.648371403	-0.120594802
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H	0.712568482	-3.286346972	-0.134605336	H	-1.301715257	2.386528421	0.798348252
C	0.700605917	-2.311646739	1.855289413	C	0.360324702	2.877417542	-0.585873284
C	2.871514390	-1.560594350	1.680347240	C	1.970327954	2.772865162	1.062012632
H	3.830510849	-1.155457830	1.955835980	H	2.919721427	2.876071279	1.560510549
O	-3.840859169	2.568378865	-1.813539323	O	-4.101033418	-3.155955269	1.508706763
C	2.592066178	-2.295969652	0.498203914	C	0.725017271	2.507114692	1.685677188
C	1.720738837	-1.571331255	2.506925659	C	1.751037928	2.986298391	-0.322195696
H	1.667746006	-1.167036445	3.503737177	H	2.505408720	3.282983532	-1.032576470
C	-0.525648389	-2.914286533	2.533589139	C	-0.353401622	3.452359479	-1.810121050
C	-1.578627731	-3.391489475	1.524729997	C	-1.800935019	2.959053547	-1.937598981
H	-1.984029570	-2.568741537	0.937878582	H	-1.852519181	1.884614829	-2.109273003
H	-2.411521897	-3.857089940	2.054731651	H	-2.281894310	3.450279146	-2.785717512
H	-1.174577523	-4.135425801	0.836375564	H	-2.390304223	3.192398933	-1.050239443
C	3.641551072	-2.899690946	-0.434703553	C	0.446615092	2.590172639	3.184714348
C	4.292789055	-4.063696645	0.353646380	C	0.427294790	4.097676656	3.538721063
H	4.799643115	-3.702960880	1.250096588	H	1.389494448	4.566624760	3.325986877
H	5.029782300	-4.572233219	-0.272251451	H	0.210595784	4.230430898	4.601267751
H	3.544599746	-4.796505708	0.660458811	H	-0.338833382	4.624965531	2.968087741
C	-1.171999112	-1.941839061	3.527113269	C	0.394325797	3.168455779	-3.120369279
H	-0.461310794	-1.600491658	4.281751994	H	1.432064424	3.502824039	-3.078976632
H	-1.994845683	-2.431688355	4.050706725	H	-0.087471529	3.699406042	-3.943887529
H	-1.578594271	-1.069554995	3.021230064	H	0.385875564	2.105929925	-3.362826171
C	-0.016729054	-4.148335948	3.319756318	C	-0.387927275	4.986540693	-1.596483976
H	0.454189808	-4.873822324	2.654136473	H	-0.913077965	5.242855292	-0.674900424
H	-0.853073689	-4.640411104	3.821580263	H	-0.907196964	5.468071489	-2.428270801
H	0.713822723	-3.861652305	4.078134712	H	0.619537307	5.402022707	-1.537536774
C	3.022877621	-3.483291720	-1.713495263	C	-0.917446413	1.994722713	3.560572014
H	2.298675351	-4.267848539	-1.488517498	H	-1.737132320	2.494284419	3.043281473
H	3.807059057	-3.930376867	-2.327670608	H	-1.087444551	2.113905097	4.632586556
H	2.525501210	-2.721259802	-2.312547923	H	-0.974913443	0.929208827	3.335047852
C	-3.839715527	1.567172234	-1.252802546	C	-4.130260470	-2.187970121	0.897803105
C	4.742946472	-1.900404742	-0.812992635	C	1.543367450	1.912761465	4.018881979
H	4.353827745	-1.096422869	-1.435611124	H	1.570202118	0.837932864	3.846254755
H	5.528685462	-2.408256455	-1.376152630	H	1.355274334	2.074954048	5.082251204
H	5.207871056	-1.454766324	0.068005633	H	2.532027960	2.320331713	3.798592777
Zr	1.203348006	-0.000002706	0.599525279	Zr	1.444254255	0.515484194	0.080728542

As	-1.412301252	0.000009611	-0.280892632	As	-0.134725718	-0.442287564	-1.948589527
As	1.690874386	-0.000014266	-2.082528310	As	-0.119018638	-1.113754572	1.637473406
As	-0.454715334	1.224179703	-2.249519669	As	-0.221642236	-2.470867680	-0.477408010
Fe	-3.896478751	0.000012363	-0.358875796	Fe	-4.212373407	-0.658688205	-0.069408121
O	-6.816773954	-0.000013597	-0.475875099	O	-7.135372790	-0.676835461	0.005300251
C	1.235650980	2.697979147	0.600088731	C	3.164885193	-1.498136411	-0.477586484
H	0.712705000	3.286344262	-0.134681395	H	2.853185098	-2.471991071	-0.815460484
C	0.700660492	2.311692339	1.855235511	C	3.498869206	-0.415856265	-1.333523725
C	2.871542818	1.560550703	1.680360290	C	3.826368274	0.205493349	0.861790556
H	3.830517199	1.155384168	1.955880849	H	4.140142384	0.776075483	1.720636367
O	-3.840828757	-2.568456649	-1.813362107	O	-4.148443995	1.959977569	1.293787906
C	2.592149211	2.295906616	0.498192009	C	3.408842863	-1.151467103	0.876360171
C	1.720745960	1.571343643	2.506908636	C	3.891904686	0.648822627	-0.482432229
H	1.667712160	1.167068804	3.503726032	H	4.255846450	1.611795625	-0.799819815
C	-0.525581495	2.914404116	2.533493696	C	3.771357659	-0.501857994	-2.833518152
C	-1.578495897	3.391684968	1.524603809	C	3.014524923	-1.660202346	-3.499354139
H	-1.983935482	2.568968887	0.937735095	H	1.932872799	-1.541222626	-3.424957522
H	-2.411374960	3.857340897	2.054580523	H	3.268228752	-1.703905767	-4.560382549
H	-1.174373382	4.135596556	0.836265241	H	3.281067143	-2.623282365	-3.061146455
C	-5.674217037	0.000012680	-0.429151273	C	-5.993083743	-0.669325404	-0.024154330
C	3.641676588	2.899564319	-0.434708193	C	3.620464592	-2.129019686	2.033029033
C	4.292934758	4.063574268	0.353619746	C	5.139434388	-2.430935351	2.064498813
H	4.799768657	3.702849811	1.250085935	H	5.720856074	-1.525905177	2.247579853
H	5.029949012	4.572075455	-0.272282094	H	5.362917461	-3.146004630	2.859721723
H	3.544760452	4.796410599	0.660403708	H	5.473490740	-2.860058745	1.118202249
C	-1.172026428	1.941992332	3.526990686	C	3.433302515	0.806975244	-3.560960431
H	-0.461387345	1.600601901	4.281656234	H	3.954461856	1.660095257	-3.122803859
H	-1.994864553	2.431888400	4.050553549	H	3.737759724	0.741933380	-4.607594108
H	-1.578653698	1.069733470	3.021089843	H	2.364096074	1.011501811	-3.536149908
C	-0.016611333	4.148416393	3.319686223	C	5.288864926	-0.768718544	-2.988046502
H	0.454378490	4.873876713	2.654088180	H	5.578761928	-1.690787960	-2.481181271
H	-0.852942262	4.640541974	3.821483572	H	5.547700970	-0.866208551	-4.045018128
H	0.713894537	3.861679140	4.078088642	H	5.879728737	0.046539863	-2.567374873
C	3.023048063	3.483141238	-1.713532433	C	2.879656576	-3.458207666	1.827171659
H	2.298866802	4.267729284	-1.488596213	H	3.181314734	-3.950209456	0.901156940
H	3.807256784	3.930179293	-2.327707195	H	3.114535121	-4.138668139	2.647991995
H	2.525659561	2.721104774	-2.312569805	H	1.798577895	-3.326596781	1.806984193
C	-3.839721253	-1.567188258	-1.252735081	C	-4.164375966	0.940180619	0.765173427
C	4.743047312	1.900230071	-0.812943209	C	3.220497584	-1.535275028	3.390842338
H	4.353919859	1.096251368	-1.435560582	H	2.145067859	-1.367084691	3.451346491
H	5.528823207	2.408042831	-1.376087171	H	3.493892522	-2.224027878	4.192854735
H	5.207926773	1.454589785	0.068077874	H	3.725274057	-0.588369413	3.587189609
O	-4.064966808	0.000042944	2.585207617	O	-4.256447151	-0.799688394	-3.021751928
C	-3.958407100	0.000062374	1.441189477	C	-4.222088783	-0.748679078	-1.878094180

**Table S13:** Cartesian coordinates of the optimized geometry of  $[\text{Cp}^*_2\text{Zr}(\mu, \eta^{3:1:1}\text{-As}_4)(\text{Fe}(\text{CO})_3)]$  at the B3LYP/def2- SVP level of theory.

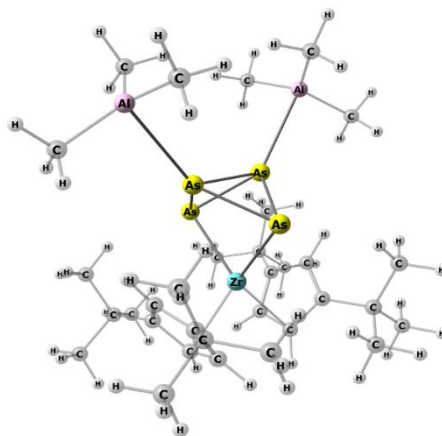
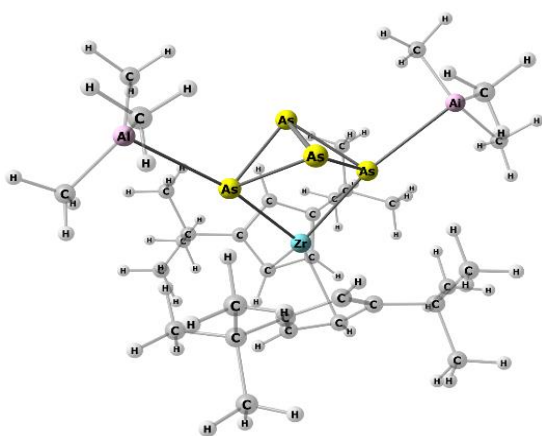
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C	-0.139333919	-3.234947504	1.537058652
H	0.213554753	-4.175642706	1.121910813
C	-0.255722635	-1.299693768	2.729000469
H	0.019274906	-0.458469045	3.357377259
C	0.645124726	-2.312074749	2.290250489
C	2.030855512	-2.589959782	2.884244559
C	-1.498152027	-2.805676734	1.557310297
H	-2.338922990	-3.362273794	1.150136693
C	-1.583828046	-1.607084846	2.323028204
C	1.802102760	-3.559084518	4.074176445
H	1.124191514	-3.117977286	4.821616883
H	2.758954595	-3.785485501	4.572932373
H	1.360124614	-4.510093459	3.738007258
C	2.699320669	-1.312303257	3.422653855
H	2.879895732	-0.576903740	2.624441776
H	3.674070850	-1.561210804	3.871525874
H	2.093805914	-0.828517526	4.203995869
C	2.974115784	-3.265494531	1.875856855
H	2.541764366	-4.187807194	1.457117660
H	3.920483522	-3.541320636	2.367765913
H	3.210260015	-2.589092381	1.043685340
C	-2.866143585	-1.005725021	2.908535165
O	-0.800126240	5.022200058	2.205778978
C	-2.629689468	0.400158578	3.488181795
H	-1.889605811	0.389494272	4.302672276
H	-3.569141230	0.798163823	3.903248780
H	-2.276611189	1.103486285	2.719562106
C	-4.006972390	-0.940828798	1.878304744
H	-3.781301000	-0.222664731	1.077630298
H	-4.939580376	-0.614933952	2.366068481
H	-4.204023762	-1.920822078	1.416287026
C	-0.384266654	4.379476199	1.350679503
C	-3.297444057	-1.945736854	4.064660912
H	-3.525269002	-2.957716449	3.695146721
H	-4.200087054	-1.552035770	4.560346697
H	-2.502837384	-2.033637603	4.821931997





Zr	-0.273288057	-1.246370651	0.000000000
As	2.084475185	0.162055181	0.000000000
As	-1.220100144	1.407541044	0.000000000
As	0.739518263	1.573521557	-1.576914515
Fe	0.280852980	3.389215245	0.000000000
C	-0.139333919	-3.234947504	-1.537058652
H	0.213554753	-4.175642706	-1.121910813
C	-0.255722635	-1.299693768	-2.729000469
H	0.019274906	-0.458469045	-3.357377259
C	0.645124726	-2.312074749	-2.290250489
C	2.030855512	-2.589959782	-2.884244559
O	3.044256890	4.323417183	0.000000000
C	-1.498152027	-2.805676734	-1.557310297
H	-2.338922990	-3.362273794	-1.150136693
C	-1.583828046	-1.607084846	-2.323028204
C	1.802102760	-3.559084518	-4.074176445
H	1.124191514	-3.117977286	-4.821616883
H	2.758954595	-3.785485501	-4.572932373
H	1.360124614	-4.510093459	-3.738007258
C	2.699320669	-1.312303257	-3.422653855
H	2.879895732	-0.576903740	-2.624441776
H	3.674070850	-1.561210804	-3.871525874
H	2.093805914	-0.828517526	-4.203995869
C	2.974115784	-3.265494531	-1.875856855
H	2.541764366	-4.187807194	-1.457117660
H	3.920483522	-3.541320636	-2.367765913
H	3.210260015	-2.589092381	-1.043685340
C	-2.866143585	-1.005725021	-2.908535165
O	-0.800126240	5.022200058	-2.205778978
C	-2.629689468	0.400158578	-3.488181795
H	-1.889605811	0.389494272	-4.302672276
H	-3.569141230	0.798163823	-3.903248780
H	-2.276611189	1.103486285	-2.719562106
C	-4.006972390	-0.940828798	-1.878304744
H	-3.781301000	-0.222664731	-1.077630298
H	-4.939580376	-0.614933952	-2.366068481
H	-4.204023762	-1.920822078	-1.416287026
C	-0.384266654	4.379476199	-1.350679503
C	1.954520985	3.957036753	0.000000000
C	-3.297444057	-1.945736854	-4.064660912
H	-3.525269002	-2.957716449	-3.695146721
H	-4.200087054	-1.552035770	-4.560346697
H	-2.502837384	-2.033637603	-4.821931997

**Table S14:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1:1}\text{-As}_4)(\text{AlMe}_3)_2]$  at the B3LYP/def2- SVP level of theory.



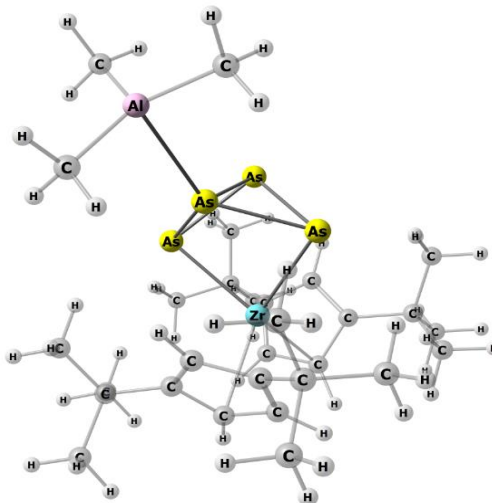
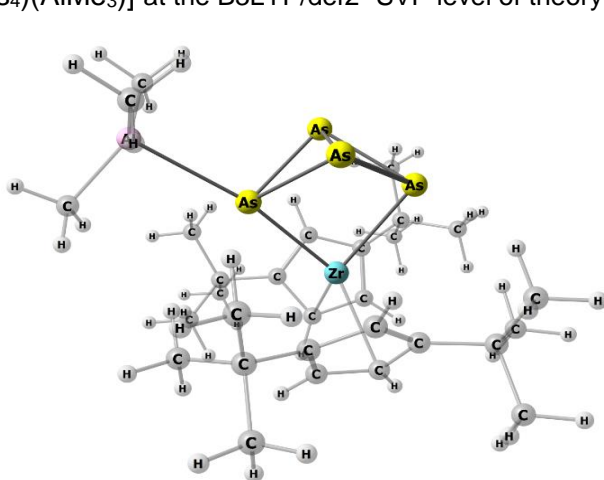
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As	0.004411473	-2.133812973	1.229491389
Al	-3.997326414	-2.638538042	0.074418289
C	0.178331886	1.194633430	-2.672594461
H	0.329272191	0.289297483	-3.255319801
C	-2.448426496	0.018311495	-3.646565297
H	-2.388438370	-0.735922059	-2.849385076
H	-1.628917784	-0.167630109	-4.357828659
H	-3.392833521	-0.146953423	-4.188141290
C	1.225678307	2.037567321	-2.196425379
C	-0.823472387	2.942548631	-1.611749920
C	-1.567590263	3.655235734	-1.261744573
C	0.586580603	3.112964306	-1.514407516
H	1.083435722	3.972939545	-1.070868048

As	-0.561874598	-0.056441055	1.828948356
As	-1.741124750	1.214006620	0.042079552
Al	-4.138158620	2.963583934	0.148611304
C	1.496845044	-2.673950901	-0.324499744
H	0.612724986	-3.260251675	-0.563909459
C	1.993726775	-2.447216093	0.991348170
C	2.390454657	-2.126140570	-1.292201851
C	3.176822273	-1.665067522	0.834872463
H	3.836594249	-1.345969789	1.639827451
C	2.447175029	-2.479069695	-2.782164071
C	3.426675703	-1.485711699	-0.554051749
H	4.306166264	-1.002261636	-0.973934375
C	1.623499861	-3.244575270	2.249946355
C	0.171738634	-3.755491210	2.229007399

C	-1.090803626	1.767663153	-2.376174158
C	-2.485208400	2.437714742	-4.287308472
H	-3.399345936	2.252838589	-4.874668452
H	-1.619217478	2.316218355	-4.956628927
H	-2.504845517	3.484593989	-3.946580089
C	-3.628031636	-3.541355647	1.805554229
H	-4.420017188	-4.291998675	1.993215081
H	-2.671383095	-4.092578790	1.821326240
H	-3.634224544	-2.859236716	2.673524241
C	3.110754208	0.624883130	-3.166391925
H	3.036221190	-0.143859071	-2.383167294
H	4.158992048	0.651884404	-3.502288443
H	2.502256120	0.297396984	-4.023348129
C	2.777436603	3.012484479	-3.843406660
H	3.800690218	3.024816844	-4.252852757
H	2.524810956	4.036347606	-3.526725510
H	2.089179920	2.730075064	-4.655274359
C	-3.646076273	-3.671941214	-1.584739199
H	-3.685511192	-3.063273853	-2.504786429
H	-2.677829432	-4.202722976	-1.576633289
H	-4.424419413	-4.451838542	-1.693039467
C	-2.411152668	1.452404135	-3.089888669
C	2.686190099	2.014083350	-2.658946361
C	-3.639737608	1.684069674	-2.194498644
H	-3.658030901	2.700824242	-1.772804401
H	-3.676797960	0.965832677	-1.363313758
H	-4.563212022	1.556292721	-2.780781458
C	3.653739114	2.475034491	-1.555165256
H	3.670527697	1.771706909	-0.712035919
H	3.389211234	3.471323885	-1.166806105
H	4.678560216	2.541462026	-1.953011406
C	-5.484939225	-1.319431238	0.042392918
H	-5.555905387	-0.750906533	-0.900986445
H	-6.443353996	-1.863123596	0.150045752
H	-5.450057819	-0.590265915	0.870696080
Zr	-0.000002370	1.198491741	-0.000006360
As	1.776123094	-0.880668737	-0.008355569
As	-0.004400878	-2.133826970	-1.229486912
Al	3.997337061	-2.638522072	-0.074400166
C	-0.178339844	1.194630260	2.672578813
H	-0.329278765	0.289291431	3.255299809
C	2.448442339	0.018330136	3.646567546
H	2.388475285	-0.735910877	2.849393326
H	1.628932649	-0.167622202	4.357826595
H	3.392848264	-0.146912904	4.188152392
C	-1.225687922	2.037567332	2.196420484
C	0.823457797	2.942550710	1.611736198
H	1.567573488	3.655240147	1.261730655
C	-0.586594870	3.112961147	1.514393890
H	-1.083453655	3.972933825	1.070853490
C	1.090793376	1.767668551	2.376164405
C	2.485197155	2.437732273	4.287294501
H	3.399323086	2.252848167	4.874670225
H	1.619193782	2.316247803	4.956600923
H	2.504851269	3.484609568	3.946561017
C	3.628070144	-3.541342264	-1.805540999
H	4.420061443	-4.291981583	-1.993192411
H	2.671424424	-4.092570133	-1.821324425
C	3.634270387	-2.859223328	-2.673511033
C	-3.110783826	0.624884331	3.166361015
H	-3.036255094	-0.143841068	2.383120133
H	-4.159023376	0.651890574	3.502251866
H	-2.502295364	0.297372766	4.023314208
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H	-3.800678598	3.024783812	4.252894287
H	-2.524806072	4.036330842	3.526778067
H	-2.089163812	2.730026221	4.655285456
C	3.646069558	-3.671923036	1.584754789
H	3.685488373	-3.063251051	2.504799647
H	2.677826574	-4.202711620	1.576638612
H	4.424417027	-4.451814179	1.693068900
C	2.411146466	1.452417603	3.089878699
C	-2.686200095	2.014090483	2.658947414
C	3.639728935	1.684095244	2.194487600
H	3.658019941	2.700854770	1.772805116
H	3.676788879	0.965868359	1.363293586
H	4.563205365	1.556313459	2.780766175
C	-3.653750910	2.475088943	1.555188058
H	-3.670554759	1.771789408	0.712036358
H	-3.389210350	3.471386539	1.166858837
H	-4.678568572	2.541519029	1.953042717
C	5.484943459	-1.319408181	-0.042347785
H	5.555886707	-0.750884731	0.901034261
H	6.443363204	-1.863095936	-0.149980489
H	5.450076975	-0.590241409	-0.870650227

H	-0.558231086	-2.934396798	2.261943888
H	-0.009928476	-4.394302730	3.107695182
H	-0.038643351	-4.364600868	1.336488949
C	3.412417763	-3.686532800	-2.910038372
H	4.421363177	-3.432757336	-2.549452481
H	3.495213274	-4.001451092	-3.963285299
H	3.051464024	-4.546627168	-2.324847913
C	2.566238634	-4.478187738	2.255872553
H	2.425594011	-5.088217174	1.350128577
H	2.356938274	-5.114125603	3.131649237
H	3.623887792	-4.174960723	2.298040873
C	1.074223068	-2.898393488	-3.335989867
H	0.658669631	-3.762917716	-2.796218040
H	1.168898816	-3.188686072	-4.394254760
H	0.340088797	-2.079987360	-3.283201119
C	1.863502625	-2.448373880	3.545063502
H	2.901663862	-2.090734230	3.623205645
H	1.671774781	-3.088151640	4.420958499
H	1.194726751	-1.577987474	3.617623503
C	3.001614517	-1.315371797	-3.623066239
H	2.347854566	-0.434177658	-3.566772501
H	3.079401350	-1.612390462	-4.681032062
H	4.009286540	-0.001512537	-3.294579266
Zr	1.475561090	0.000251885	0.000282186
As	-0.559947588	0.055645371	-1.830450066
As	-1.740325788	-1.215606238	-0.044866230
Al	-4.138275569	-2.963636921	-0.148607791
C	1.495182956	2.674042189	0.325207145
H	0.610470299	3.259720715	0.563963388
C	1.993320795	2.447771956	-0.990258028
C	2.388364592	2.126718527	1.293592619
C	3.176757031	1.666330854	-0.832874051
H	3.837372521	1.347692959	-1.637321082
C	2.443806085	2.479771035	2.783581928
C	3.425591387	1.487020778	0.556228160
H	4.305054510	1.004111973	0.976790128
C	1.623804789	3.245155381	-2.249066010
C	0.171755699	3.755303199	-2.229425163
H	-0.557770484	2.933856598	-2.263337228
H	-0.009359221	4.394274239	-3.108110300
H	-0.039839088	4.364043332	-1.336942697
C	3.408038683	3.687985445	2.912012119
H	4.417397940	3.435006551	2.552024939
H	3.489961603	4.002974238	3.965307428
H	3.046747356	4.547795623	3.26611951
C	2.565869877	4.479292586	-2.253817070
H	2.424009755	5.089042236	-1.348075269
H	2.357060906	5.115310970	-3.129651344
H	3.623728345	4.176666886	-2.295030246
C	1.070195310	2.898099911	3.336495269
H	0.654256171	3.762176164	2.796306122
H	1.163996655	3.188674134	4.394760934
H	0.336770369	2.079095490	3.283429718
C	1.865494776	2.449363462	-3.544121921
H	2.903893804	2.092198485	-3.621285653
H	1.674387355	3.089270807	-4.420057691
H	1.197173836	1.578704589	-3.617601055
C	2.998590502	1.316537728	3.624898526
H	2.345627899	0.434781246	3.568096597
H	3.075314551	1.613616053	4.682924817
H	4.006770879	1.017446361	3.297180691
C	-4.591656718	2.797852621	-1.769870182
H	-3.802498756	3.176717840	-2.441878530
H	-4.822254499	1.761952982	-2.071288321
H	-5.498694130	3.396332939	-1.982300668
C	-5.151305850	1.919587042	1.488305499
H	-6.118129332	2.422053159	1.685203759
H	-5.392036233	0.897766703	1.149399751
H	-4.636399824	1.839700518	2.460908051
C	-3.141120488	4.567856034	0.756612455
H	-2.389649530	4.918225937	0.027715868
H	-3.850079447	5.406180611	0.899181389
H	-2.634177590	4.423754989	1.726727700
C	-3.144110049	-4.569067041	-0.758185863
H	-2.394934672	-4.923084530	-0.028697161
H	-3.855009628	-5.405155013	-0.904181199
H	-2.634915448	-4.424117809	-1.727006164
C	-5.152692162	-1.919024108	-1.486905719
H	-6.118911879	-2.422322404	-1.684621156
H	-5.394549189	-0.897975331	-1.146489932
H	-4.637867243	-1.837151154	-2.459389826
C	-4.588632433	-2.797428268	1.770593621
H	-4.820660014	-1.761806886	2.071851556
H	-5.494112725	-3.397587628	1.984945163
H	-3.797589441	-3.174438477	2.441433540

**Table S15:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1}\text{-As}_4)(\text{AlMe}_3)]$  at the B3LYP/def2- SVP level of theory.



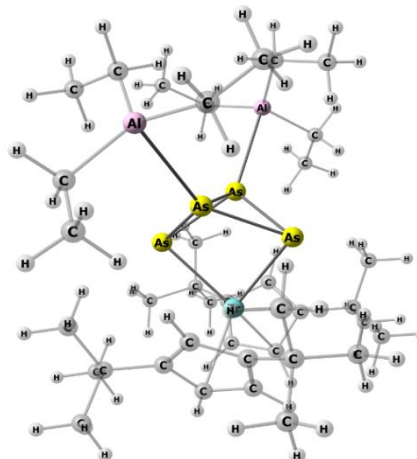
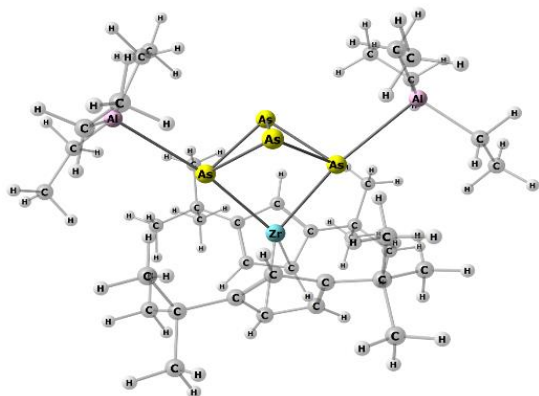
As	1.287504482	-0.031353714	-2.123954713
As	-0.941737221	1.072696942	-2.321526140
C	0.734600936	-2.593766948	0.843503233
H	0.093437601	-3.235099912	0.243876550
C	2.219963389	-3.748220474	-1.552320669
H	1.717844730	-3.021105607	-2.205393959
H	1.459772833	-4.442569024	-1.162394889
H	2.909618211	-4.337867902	-2.176915143
C	0.369508105	-2.033364558	2.103781497
C	2.543366927	-1.431840424	1.591909768
H	3.551875912	-1.036725997	1.698163702
C	1.502502515	-1.297347094	2.551837589
H	1.589710941	-0.774940319	3.502131785
C	2.091310716	-2.284075689	0.540299518
C	3.665395164	-4.172027017	0.442877658
H	4.316265098	-4.804349120	-0.183390521
H	2.905906821	-4.819540608	0.908145885
H	4.280494754	-3.741713102	1.248334623
C	-1.974654708	-3.024784934	2.123531387
H	-2.355690998	-2.299890157	1.389563575
H	-2.816019043	-3.309442161	2.774349261
H	-1.663256752	-3.928989682	1.578258254
C	-0.318106271	-3.549894879	3.925935942
H	-1.141862229	-3.913483640	4.561897223
H	0.481412327	-3.175934086	4.584395088
H	0.081731259	-4.407673494	3.362933245
C	3.003331443	-3.062936397	-0.418455596
C	-0.828028232	-2.441712670	2.967526416
C	4.119041574	-2.192609640	-1.023412718
H	4.711775979	-1.684252516	-0.247656490
H	3.713361224	-1.428286056	-1.702435056
H	4.811921953	-2.821041856	-1.605501410
C	-1.358165245	-1.269907375	3.813238514
H	-1.776558395	-0.471674285	3.185263719
H	-0.569494147	-0.831903874	4.445579206
H	-2.158319314	-1.617963958	4.485537391
Zr	0.796232803	0.073229501	0.556943280
As	-1.792196853	-0.091179058	-0.270969732
As	-0.822953460	-1.369330567	-2.189573560
Al	-4.572770054	-0.292605516	-0.575140945
C	0.904061451	2.749961937	0.311780939
H	0.583034015	3.278641548	-0.581901094
C	-2.002777970	3.660477356	0.530183490
H	-2.328623878	2.806579558	-0.079739258
H	-1.401372456	4.327983469	-0.106305291
H	-2.905315640	4.218551757	0.824811359
C	2.235398230	2.298392813	0.553946015
C	0.906065446	1.805949836	2.383888261
H	0.606777335	1.496324116	3.383432656

As	-0.512646515	-0.269833241	-2.010681174
As	-0.515440055	-2.471310438	-0.812143173
C	-0.892919026	2.276917207	0.995245047
H	-1.939596461	2.020377966	1.139840259
C	-0.348382821	2.834386431	-0.196466105
C	0.107038087	2.202914891	2.009239315
C	1.041503319	3.029697228	0.060611383
H	1.756807548	3.480305155	-0.624969756
C	-0.136178486	2.056313833	3.515386347
C	1.313990518	2.660429417	1.406956790
H	2.272181764	2.781418423	1.907521171
C	-1.141762749	3.510175893	-1.323869548
C	-2.546778824	2.908871753	-1.506161564
H	-2.508602627	1.862326740	-1.838814257
H	-3.099706791	3.479576081	-2.268999789
H	-3.136728486	2.951537712	-0.577716074
C	-0.245491920	3.496456825	4.082297067
H	0.685566187	4.062527412	3.923503415
H	-0.446776327	3.467669313	5.165967420
H	-1.064277822	4.051659567	3.598624732
C	-1.306786447	4.991783860	-0.890688301
H	-1.842310494	5.065772338	0.068627036
H	-1.883149696	5.549866363	-1.646972423
H	-0.330271928	5.486363823	-0.771448352
C	-1.451029153	1.318161101	3.823245938
H	-2.323055071	1.839120984	3.399272571
H	-1.602924285	1.261011599	4.912781936
H	-1.448190307	0.289051365	3.433637585
C	-0.397770921	3.481766949	-2.670798904
H	0.604197115	3.931826167	-2.597116047
H	-0.960044240	4.056948423	-3.423455114
H	-0.286007229	2.455892536	-3.051809043
C	1.028804320	1.340926126	4.223212867
H	1.130436885	0.300497302	3.884951948
H	0.859502907	1.326068205	5.311820793
H	1.989094558	1.852585709	4.050809729
Zr	0.955790337	0.507620811	0.152687729
As	-0.468457693	-1.408814249	1.465500420
As	-2.177329012	-0.789166461	-0.232353847
Al	-5.042577536	-1.316326761	-0.316626216
C	2.846181151	-1.217105159	-0.696070816
H	2.616355720	-2.140715482	-1.221537569
C	3.035075394	-1.107313707	0.711276258
C	3.110517284	0.033230858	-1.329736785
C	3.339908520	0.263799908	0.961305491
H	3.584185131	0.693697821	1.931006650
C	3.412974896	0.255882682	-2.815113324
C	3.401737235	0.952174670	-0.281111010
H	3.695413241	1.991967953	-0.406550897

C	2.218150121	1.697610965	1.845667595
H	3.078984602	1.288738984	2.370728374
C	0.084953804	2.505574479	1.449651800
C	-0.831403388	4.489390891	2.579035500
H	-1.729303423	5.070834681	2.845394339
H	-0.170209781	5.136765710	1.981951184
H	-0.302512424	4.233746759	3.510401677
C	-4.691367417	-2.102791396	-1.389028000
H	-5.755848184	-2.348004106	-1.569869356
H	-4.184442622	-2.181024823	-2.366843361
H	-4.292566684	-2.904102676	-0.742598831
C	3.164025926	3.187661357	-1.643436423
H	2.697915582	2.388631567	-2.239263891
H	4.087159115	3.494591427	-2.160112516
H	2.484910817	4.054085987	-1.644763018
C	4.093889044	3.924412346	0.561409171
H	4.986928389	4.307652659	0.040686873
H	4.392284125	3.636585130	1.581473504
H	3.367071321	4.747672712	0.642926767
C	-4.903049318	1.266857049	-1.762939484
H	-4.619508846	2.233410524	-1.310785439
H	-4.389712286	1.192969147	-2.737823706
H	-5.985636261	1.331821182	-1.985359805
C	-1.232432947	3.215970943	1.786189263
C	3.492626233	2.722628953	-0.213680415
C	-2.153870362	2.363016393	2.674706937
H	-1.652015556	2.045130941	3.601451338
H	-2.509233348	1.464841145	2.149549233
H	-3.041055314	2.946226979	2.967518240
C	4.546590904	1.602175505	-0.272497200
H	4.193998547	0.747336555	-0.865751728
H	4.812715682	1.236133902	0.731835456
H	5.472149329	1.975902381	-0.739144748
C	-5.145990265	-0.133335465	1.324091987
H	-4.975670492	0.866081993	1.760457913
H	-6.236148135	-0.317381133	1.383580512
H	-4.671957582	-0.873893120	1.991886608

C	3.311842165	-2.263507692	1.682925524
C	2.673555791	-3.587567389	1.225586045
H	1.575703630	-3.535610687	1.214194674
H	2.961043397	-4.397096087	1.915183668
H	3.013324347	-3.881148751	0.220244086
C	4.951310622	0.133419282	-2.971901315
H	5.476064658	0.895772647	-2.375391039
H	5.241959104	0.265704356	-4.027281837
H	5.306339470	-0.855468459	-2.642096680
C	4.852763684	-2.450542496	1.688630558
H	5.228856157	-2.674420900	0.678149704
H	5.134921808	-3.285495986	2.351128829
H	5.365293837	-1.543697090	2.045461317
C	2.751563222	-0.808028333	-3.708880500
H	3.086916334	-1.824762252	-3.452288612
H	3.018741095	-0.632251658	-4.763021641
H	1.653668410	-0.783804874	-3.635823776
C	2.859525144	-1.951506479	3.120685822
H	3.307062642	-1.020173296	3.500025723
H	3.169605581	-2.763082395	3.798115215
H	1.765579761	-1.859461245	3.191438307
C	2.982895009	1.656734674	-3.285616173
H	1.895072726	1.790554409	-3.210304365
H	3.270619385	1.810310257	-4.337930239
H	3.466190633	2.452461144	-2.696866837
C	-5.576440428	0.219199364	0.821846791
H	-5.317553371	1.199893791	0.385782139
H	-6.676247390	0.216094108	0.949142315
H	-5.146793746	0.176144929	1.837841423
C	-4.983178422	-3.117426857	0.503983812
H	-6.012941066	-3.515935781	0.586872381
H	-4.410101840	-3.845948637	-0.094498576
H	-4.564122879	-3.117446617	1.524835509
C	-5.258090998	-1.154999954	-2.279167491
H	-4.675007961	-1.901728109	-2.844654814
H	-6.320955722	-1.322521749	-2.540829532
H	-4.993883022	-0.157183470	-2.669524323

**Table S16:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}^*_2\text{Zr}(\mu, \eta^{1:1:1:1}\text{-As}_4)(\text{AlEt}_3)_2]$  at the B3LYP/def2- SVP level of theory.



As	1.789479893	0.610237842	-0.036213091
As	-0.022145310	1.849806301	-1.226861404
Al	4.016914730	2.441809060	-0.087343100
C	-0.237659840	-1.502037760	2.673848347
H	-0.462944310	-0.618770175	3.266554859
C	1.071694585	-1.993504383	2.407564307
C	-1.216930621	-2.403377388	2.157938386
C	0.898299293	-3.171471550	1.621040510
H	1.696872139	-3.826204420	1.277363054
C	-2.693507710	-2.472121465	2.558304685
C	-0.494346371	-3.430183291	1.487394626
H	-0.924926048	-4.311627273	1.017604548
C	2.350620427	-1.624056836	3.168894277
C	2.341317152	-0.173420242	3.681005607
H	2.340249939	0.555606885	2.859334460
H	3.241859099	0.013563655	4.286414046
H	1.470243388	0.030552432	4.322763014
C	-2.774920275	-3.462023372	3.750102794

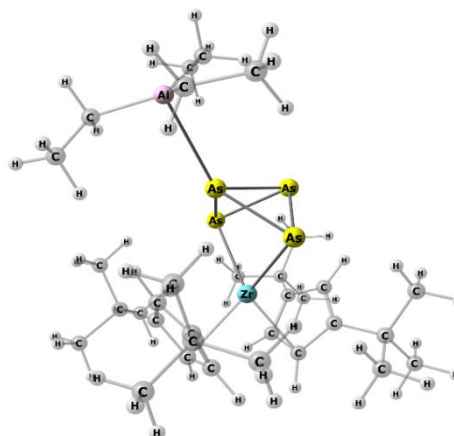
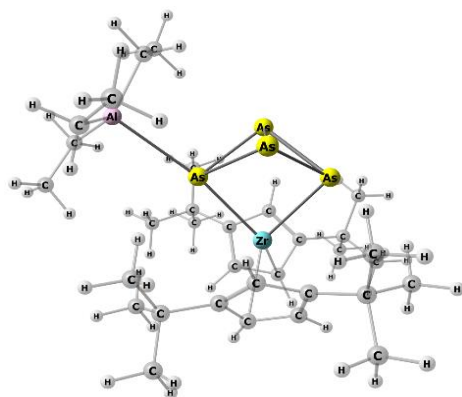
As	0.183572246	-0.126844455	1.823585526
As	1.370336877	-1.215327462	-0.075460724
Al	3.666100663	-3.193206458	0.193291734
C	-1.862711145	2.687074846	0.038614387
H	-0.966556189	3.290140707	-0.083956544
C	-2.406927056	2.284079632	1.292367351
C	-2.723871022	2.289037710	-1.026216071
C	-3.586926735	1.542675741	0.987688343
H	-4.277966514	1.122981275	1.716607101
C	-2.727353511	2.854232366	-2.450560959
C	-3.786302937	1.557884761	-0.420844663
H	-4.652411288	1.146186401	-0.934225867
C	-2.076190481	2.894153646	2.661868784
C	-0.641024390	3.445215835	2.733454586
H	0.113414144	2.653468498	2.622839904
H	-0.474922430	3.926928647	3.709899548
H	-0.453576679	4.205950740	1.960645894
C	-3.667203961	4.088524377	-2.426358212

H	-2.426600416	-4.466311503	3.462882142	H	-4.691740720	3.807100836	-2.137113790
H	-3.815549436	-3.549273509	4.102743094	H	-3.710178001	4.556601011	-3.423551842
H	-2.157158469	-3.118739714	4.594529139	H	-3.309653097	4.844776415	-1.710358470
C	2.387324309	-2.568512048	4.401046803	C	-3.056202912	4.085402311	2.838238053
H	1.499230908	-2.427459895	5.036482166	H	-2.937612471	4.820181738	2.026660565
H	3.280937076	-2.360257263	5.011695355	H	-2.864415859	4.599832813	3.794309478
C	2.420806401	-3.625976925	4.096147614	H	-4.104231300	3.747565008	2.837094167
C	-3.233093754	-1.109593911	3.023837019	C	-1.330748296	3.321762318	-2.897227171
H	-2.672740006	-0.718871444	3.886905390	H	-0.922791352	4.098104956	-2.232442680
H	-4.284826540	-1.206902728	3.334756112	H	-1.385378053	3.754332608	-3.908708217
H	-3.195924291	-0.354046320	2.225456905	H	-0.607586749	2.492461843	-2.932111038
C	3.620505926	-1.868015650	2.336169252	C	-2.300219294	1.909643817	3.823177230
H	3.690333806	-2.909878767	1.987598907	H	-3.319261209	1.493776117	3.821336804
H	4.515747236	-1.667170960	2.944772408	H	-2.159382506	2.426143064	4.785840352
H	3.666382699	-1.207674332	1.458946528	H	-1.587304412	1.072474138	3.789330222
C	-3.571840870	-3.007410854	1.413580411	C	-3.277681096	1.840347130	-3.469393954
C	-3.552414832	-2.335052874	0.544975830	H	-2.639177315	0.948879981	-3.538278677
H	-4.618034230	-3.095913627	1.745964336	H	-3.327753414	2.296761137	-4.470771440
H	-3.249973995	-4.007303194	1.081728374	H	-4.296685837	1.511439800	-3.211094379
C	3.310208982	3.403050500	-2.907652873	C	4.674040884	-1.722456139	2.641944425
H	3.654447752	3.569280938	-3.944933681	H	5.459556762	-1.096764019	3.101697979
H	3.064880043	4.394573880	-2.490252528	H	4.619397390	-2.653489749	3.231873863
H	2.356687280	2.850221277	-2.978494535	H	3.716619358	-1.196336603	2.797762936
C	3.157697225	3.987400997	2.390978701	C	1.641476081	-5.440507651	0.551914164
H	2.766469637	4.927976996	2.819576067	H	1.149840016	-6.159419498	1.232260473
H	4.158314844	3.828042718	2.828191437	H	2.147098116	-6.033599881	-0.228835845
H	2.516268723	3.17555573	2.777554440	H	0.835849170	-4.884276247	0.040883395
C	6.181176938	0.313610479	0.165323044	C	4.691603441	-2.535429882	-2.589279234
H	6.683086795	0.720787018	-0.728941406	H	5.692812273	-2.328026458	-2.174769133
H	5.526816620	-0.501135740	-0.191601783	H	4.166223462	-1.566511604	-2.634711651
C	6.965704224	-0.159691296	0.784029414	H	4.839608232	-2.866978997	-3.632789146
C	5.394473623	1.398190937	0.917791654	C	3.925489095	-3.565175518	-1.742883577
H	6.103571983	2.169401096	1.284564580	H	4.462628096	-4.537040916	-1.771108314
H	4.956887700	0.977881783	1.842249882	C	2.947230119	-3.789548857	-2.209246640
C	4.340648919	2.657439147	-2.046173394	C	4.935679816	-2.003803579	1.153418492
H	5.300230224	3.217490465	-2.070769320	H	5.924696262	-2.495984507	1.039392918
H	4.589577321	1.685008562	-2.509895307	H	5.045095796	-1.053763536	0.598024077
C	3.201759475	4.001903401	0.854779624	C	2.614754329	-4.498000473	1.275272497
H	2.195742396	4.221914663	0.449534224	H	3.382825097	-5.101608312	1.803011395
Zr	0.001064187	-1.465709212	0.000663721	Zr	-1.854230656	0.000071365	-0.000070774
As	-1.790339764	0.607591205	0.036231443	As	0.183617792	0.126932303	-1.823650768
As	0.019416190	1.849910490	1.227014532	As	1.370365506	1.215358202	0.075471168
Al	-4.020752869	2.437751419	0.085335449	Al	3.666072866	3.193076264	-0.193157589
C	0.240050955	-1.503124213	-2.672493288	C	-1.862823511	-2.687136045	-0.038517357
H	0.464348510	-0.619892131	-3.265632021	H	-0.966716456	-3.290252617	0.084187770
C	-1.068762986	-1.995990251	-2.406153526	C	-2.406878086	-2.284202173	-1.292347068
C	1.220298119	-2.403055870	-2.155947505	C	-2.724061775	-2.288928213	1.026192592
C	-0.894124217	-3.173286861	-1.618898935	C	-3.586822455	-1.542629682	-0.987863008
H	-1.691997035	-3.828742391	-1.274959960	H	-4.277854773	-1.123092254	-1.716878738
C	2.696997687	-2.470481217	-2.556124888	C	-2.727727174	-2.854078344	2.450550100
C	0.498805346	-3.430331095	-1.484957442	C	-3.786367173	-1.557747900	0.420650641
H	0.930342542	-4.311040632	-1.014675763	H	-4.652476758	-1.145911361	0.933909228
C	-2.347984039	-1.628490225	-3.167936381	C	-2.076019213	-2.894281056	-2.661808495
C	-2.340306609	-0.178144109	-3.680895914	C	-0.640857012	-3.445353157	-2.733247519
H	-2.340262962	0.551386554	-2.859667895	H	0.113574460	-2.653619737	-2.622482524
H	-3.240967192	0.007409769	-4.286567539	H	-0.474617674	-3.927014522	-3.709694650
H	-1.469369055	0.026503937	-4.322621470	H	-0.453540888	-4.206128745	-1.960451866
C	2.779381589	-3.460396528	-3.747847547	C	-3.667457050	-4.088462013	2.426237803
H	2.431676887	-4.464904812	-3.460651745	H	-4.691978924	-3.807140206	2.136843799
H	3.820154802	-3.546952897	-4.100230370	H	-3.710529348	-4.556521746	3.423435349
H	2.161589074	-3.117579398	-4.592440493	H	-3.309734399	-4.844693667	1.710303070
C	-2.383294847	-2.573711337	-4.399548390	C	-3.056030750	-4.085530964	-2.838270856
H	-1.495170944	-2.432043544	-5.034803288	H	-2.937546964	-4.820284917	-2.026655326
H	-3.276962823	-2.366787448	-5.010564689	H	-2.864131383	-4.599898904	-3.794303991
H	-2.415694681	-3.631036087	-4.094044341	H	-4.104053681	-3.747681089	-2.837264652
C	3.235579336	-1.107559420	-3.021626889	C	-1.331142518	-3.321461883	2.897455956
H	2.674519740	-0.716813796	-3.884218905	H	-0.923040378	-4.097835214	2.232793519
H	4.287161038	-1.204282962	-3.333246872	H	-1.385880337	-3.753946759	3.908966937
H	3.198647749	-0.352289103	-2.222983155	H	-0.608043815	-2.492109411	2.932355073
C	-3.617758110	-1.873448464	-2.335341889	C	-2.299955828	-1.909788669	-3.823152337
H	-3.686290913	-2.915101408	-1.985887786	H	-3.318988127	-1.493897786	-3.821375418
H	-4.513102593	-1.674330590	-2.944364492	H	-2.159082467	-2.426330525	-4.785787159
H	-3.664775016	-1.212395196	-1.458720204	H	-1.587028066	-1.072631674	-3.789314685
C	3.575644829	-3.004895252	-1.411241252	C	-3.278326491	-1.840211449	3.469242350
H	3.555357597	-2.332506298	-0.542677312	H	-2.639919872	-0.948688234	3.538224415
H	4.621987507	-3.092352587	-1.743433826	H	-3.328560833	-2.296591345	4.470627742
H	3.254737691	-4.005100187	-1.079407900	H	-4.297310869	-1.511402726	3.210729104
C	-3.316757635	3.421490660	2.897108043	C	1.641274110	5.440504000	-0.551178047
H	-3.658509150	3.589065378	3.934989488	H	1.150013104	6.159861837	-1.231317108
H	-3.084682909	4.413601274	2.473553938	H	2.146435136	6.033068693	0.230268515
H	-2.356621286	2.880114198	2.966570992	H	0.835363793	4.883894229	-0.040993244
C	-3.164919066	3.977486697	-2.398161954	C	4.693139229	2.534962772	2.588719984
H	-2.775098491	4.917436293	-2.829407354	H	4.841595626	2.866266164	3.632252158
H	-4.165580967	3.815763456	-2.834411609	H	5.694223271	2.328296487	2.173533002
H	-2.522704852	3.165645674	-2.782988725	H	4.168427676	1.565688379	2.634203138
C	-6.179414884	0.302795915	-0.160150394	C	4.673225274	1.722243140	-2.642179364
H	-6.679731441	0.709003087	0.735450795	H	4.618162185	2.653139011	-3.232294606
H	-5.521983167	-0.510208892	0.195075191	H	3.715831667	1.195915119	-2.797454219

H	-6.964565434	-0.172677011	-0.776398927
C	-5.397589683	1.389015961	-0.915308077
H	-6.109731659	2.157976122	-1.280944293
H	-4.960994984	0.969277176	-1.840494093
C	-4.342069332	2.659508326	2.043827578
H	-5.307831167	3.208776943	2.068779391
H	-4.578296675	1.687007285	2.514010681
C	-3.208078746	3.995892953	-0.862009207
H	-2.202013437	4.217833468	-0.457902324
H	-3.823539584	4.857491137	-0.527959314
H	3.816714272	4.863164938	0.518942802

H	5.458645943	1.096587692	-3.102147521
C	4.935504357	2.003959549	-1.153840236
H	5.924421936	2.496452231	-1.040389920
H	5.045456557	1.054059669	-0.598312362
C	2.614956126	4.498481479	-1.274607813
H	3.383256392	5.102413174	-1.801646604
H	2.093881930	3.963949364	-2.091560620
C	3.925831456	3.564463886	1.743111552
H	2.947613074	3.787895474	2.210009930
H	4.462254243	4.536715377	1.771455724
H	2.093236725	-3.963039586	2.091664688

**Table S17:** Cartesian coordinates of the optimized geometry of the Isomers for [Cp<sup>''</sup><sub>2</sub>Zr(μ,η<sup>1:1</sup>-As<sub>4</sub>)(AlEt<sub>3</sub>)] at the B3LYP/def2- SVP level of theory.



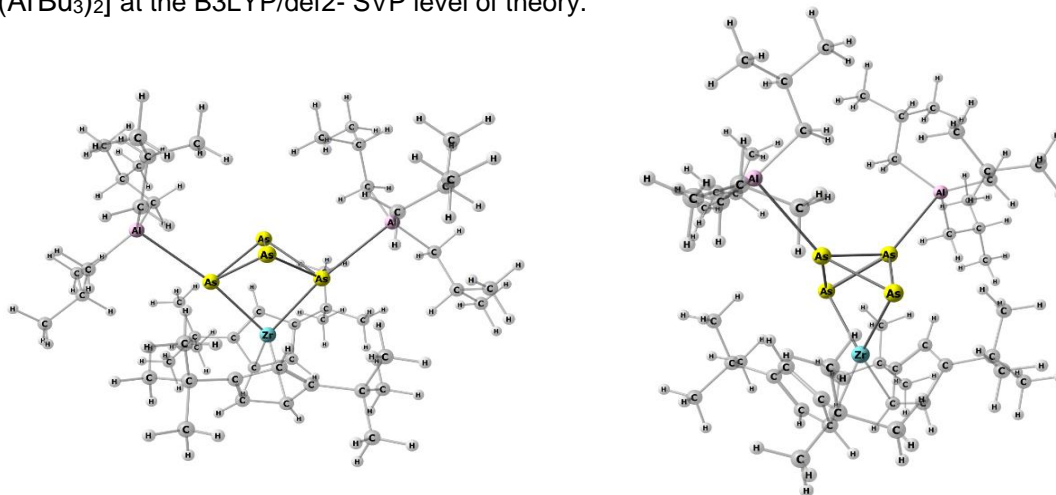
As	-1.439685180	-0.083500557	-2.154151752
As	0.751221039	1.111538267	-2.228349430
C	-0.948770267	-2.598466370	0.872783472
H	-0.241432130	-3.220514454	0.330057659
C	-2.293424838	-2.351294170	0.473135783
C	-0.695054208	-2.005421158	2.145574075
C	-2.850687921	-1.503530346	1.476823448
H	-3.878730802	-1.147822194	1.506627615
C	0.461037337	-2.339348316	3.093194572
C	-1.885280280	-1.313355325	2.503791919
H	-2.059909857	-0.783314311	3.437659300
C	-3.106469073	-3.182178748	-0.529710601
C	-2.227988256	-3.826293962	-1.617033638
H	-1.740297525	-3.073809243	-2.251839640
H	-2.848834462	-4.461484189	-2.268675430
H	-1.446310860	-4.470120039	-1.185124882
C	-0.066013525	-3.423366980	4.068957662
H	-0.909980320	-3.048824229	4.668942759
H	0.733427612	-3.734328401	4.761302212
H	-0.409822457	-4.315523456	3.522613898
C	-3.752401381	-4.322773788	0.302193301
H	-2.984965923	-4.927979922	0.809394653
H	-4.335759269	-4.990212378	-0.353490324
H	-4.429890037	-3.922965268	1.072574253
C	1.669388773	-2.915905064	2.336907375
H	1.417393435	-3.852883092	1.816880633
H	2.485144724	-3.141315374	3.041255819
H	2.062500370	-2.210244885	1.590995445
C	-4.234802558	-2.376613836	-1.197802937
H	-4.901686798	-1.910274628	-0.456738601
H	-4.852974662	-3.042451575	-1.820855468
H	-3.837786914	-1.584659960	-1.850056776
C	0.905901671	-1.115209624	3.913785562
H	1.327760382	-0.329196001	3.272014423
H	1.681581261	-1.405697279	4.639929589
H	0.070305858	-0.680482455	4.485088902
Zr	-1.094280072	0.057079747	0.543040047
As	1.555624301	-0.020550746	-0.134692181
As	0.724562126	-1.331320517	-2.102753983
Al	4.386564618	-0.149001851	-0.372229507
C	-1.338223576	2.725818294	0.245358154
H	-1.005424692	3.257070875	-0.642429197
C	-0.561444541	2.544575155	1.423238949
C	-2.653580752	2.206975136	0.435982822
C	-1.385160862	1.813790026	2.331363392
H	-1.117895088	1.539408987	3.350192598
C	-3.896359718	2.548818008	-0.392746665
C	-2.663349502	1.627061674	1.736776056
H	-3.524680515	1.182501698	2.230654145

As	-0.306723353	-0.363632174	-1.953216822
As	-0.477699612	-2.421348374	-0.536178656
C	-0.357725580	2.518026364	0.732490868
H	-1.424388798	2.389983160	0.897091647
C	0.235614027	2.891517444	-0.507241738
C	0.633384161	2.449850014	1.755703631
C	1.638884340	2.970123644	-0.263108855
H	2.392683340	3.276445600	-0.986121862
C	0.381002892	2.491656144	3.266684047
C	1.878210249	2.715725365	1.115778585
H	2.845575704	2.793860566	1.607086302
C	-0.490973266	3.517566785	-1.705602034
C	-1.960441917	3.070595613	-1.801153855
H	-2.051297984	1.989410345	-1.976129350
H	-2.453992858	3.585962622	-2.640256926
H	-2.526241306	3.317874913	-0.889954591
C	0.395341471	3.989588076	3.669700566
H	1.369313856	4.454000025	3.450111122
H	0.200525863	4.098030644	4.749507296
H	-0.377806131	4.554281696	3.125791398
C	-0.467933193	5.049898577	-1.459541784
H	-0.958364335	5.306038315	-0.507466285
H	-1.000021872	5.575275126	-2.269695827
H	0.562920517	5.435152484	-1.421938295
C	-0.990402805	1.903830313	3.643823063
H	-1.816941197	2.441997643	3.155307651
H	-1.146822975	1.983709650	4.731347933
H	-1.072185170	0.840097501	3.373380722
C	0.214254626	3.232526428	-3.043390997
H	1.271789378	3.537755664	-3.025513675
H	-0.275693268	3.794187270	-3.854652719
H	0.169262695	2.165030621	-3.304302559
C	1.482575657	1.763027211	4.056740615
H	1.496055797	0.688070285	3.831246288
H	1.312773839	1.878013385	5.139219500
H	2.482508479	2.171040434	3.839359528
Zr	1.291274663	0.490107170	0.087420606
As	-0.274213925	-1.141746858	1.615100739
As	-1.970290456	-0.544340998	-0.104639298
Al	-4.884256176	-0.850454944	-0.096106895
C	2.970160898	-1.524689440	-0.547234539
H	2.630147894	-2.488298975	-0.918360747
C	3.231252005	-1.227802726	0.820599901
C	3.319412236	-0.415146841	-1.371366212
C	3.674884397	0.128053949	0.850193509
H	4.009403096	0.667506203	1.734368787
C	3.577989026	-0.452130126	-2.881489202
C	3.741895070	0.616763275	-0.483766479
H	4.128718506	1.591026820	-0.775247353



C	0.695929351	3.332814492	1.808627748	C	3.433955129	-2.252765764	1.944464791
C	1.484365478	3.819037376	0.579551166	C	2.672733333	-3.565434169	1.684423964
H	1.863020402	2.983948008	-0.025606399	H	1.584912023	-3.412283913	1.646453316
H	2.352716794	4.413615794	0.903541836	H	2.881047820	-4.284360372	2.492546210
H	0.872694756	4.463677380	-0.070742586	H	2.984991091	-4.037725599	0.740254703
C	-4.591515078	3.734216533	0.326834517	C	5.097356251	-0.709436658	-3.059911604
H	-4.912797261	3.455943623	1.342567947	H	5.697071779	0.100568529	-2.616488390
H	-5.483224056	4.054343337	-0.236975489	H	5.352089171	-0.775598001	-4.130654019
H	-3.913992005	4.598067340	0.412822461	H	5.398368262	-1.653209528	-2.578810780
C	0.191896187	4.581883560	2.580429406	C	4.952315598	-2.574125693	1.959415715
H	-0.488181317	5.185568352	1.959217713	H	5.283069424	-2.969399301	0.986201201
H	1.043191898	5.218649333	2.872443133	H	5.175877539	-3.331193553	2.729222645
H	-0.349893884	4.297120540	3.495754633	H	5.551324088	-1.676878510	2.179615217
C	-3.534683335	2.998723664	-1.819393801	C	2.813516728	-1.595244024	-3.573051750
H	-2.894934479	3.894576825	-1.815018495	H	3.102059074	-2.580271817	-3.174816950
H	-4.450737515	3.253876619	-2.375403697	H	3.039895982	-1.599850528	-4.651060743
H	-3.012639374	2.20995600	-2.381717089	H	1.723456543	-1.490015085	-3.463335568
C	1.627442988	2.534763849	2.735616640	C	3.042697711	-1.701968428	3.327023430
H	1.108932905	2.198128022	3.646387551	H	3.573426026	-0.766914859	3.562974622
H	2.475465336	3.161095040	3.053551226	H	3.299659669	-2.431779998	4.111284708
H	2.041447593	1.651858078	2.229317089	H	1.962087733	-1.507556861	3.393706722
C	-4.884561225	1.371013854	-0.464428200	C	3.223896547	0.882380514	-3.561264755
H	-4.448927660	0.513216508	-0.994745392	H	2.145850205	1.087079848	-3.508906561
H	-5.798649046	1.672218051	-1.000921822	H	3.511805611	0.856418502	-4.624459315
H	-5.191940482	1.033368955	0.538094108	H	3.754351405	1.730085631	-3.099561034
C	4.344301719	-3.042778929	-1.357085157	C	-4.992081099	1.801854476	1.392128190
H	4.683791065	-0.084548372	-1.208297078	H	-5.255150387	2.350608769	2.314726350
H	4.766944337	-2.703350777	-2.318242077	H	-5.588550702	2.243185502	0.575575304
H	3.249677153	-3.084831857	-1.496651349	H	-3.936469597	2.042995457	1.171614183
C	4.635090396	2.159543508	-2.342504917	C	-4.844351004	-0.880210893	-3.133011895
H	4.882519495	2.496778622	-3.365895192	H	-5.132135642	-0.387015196	-4.079238771
H	5.353688292	2.648030148	-1.662071818	H	-5.328278629	-1.871859445	-3.129560410
H	3.643156400	2.582699783	-2.104395010	H	-3.756818022	-1.060709686	-3.186433873
C	4.946076921	0.338542331	2.579062594	C	-4.606439612	-3.423413166	1.484202248
H	5.533078215	-0.595145189	2.614930651	H	-5.218707093	-2.996993524	2.297289515
H	3.921535050	0.071695967	2.892979524	H	-3.553222081	-3.221413002	1.745904708
H	5.353842812	1.002647221	3.363543534	H	-4.740096249	-4.519688035	1.524288885
C	4.972220987	0.971078003	1.178796129	C	-4.977574223	-2.827893431	0.116503433
H	6.016643666	1.253198868	0.929790795	H	-6.026511552	-3.095972318	-0.130741458
H	4.429883518	1.935241608	1.186772624	H	-4.379764929	-3.307168879	-0.681284566
C	4.736531192	-2.111064082	-0.200656892	C	-5.214627538	0.286248990	1.510259708
H	5.837940827	-2.154948598	-0.061157306	H	-6.274135442	0.094373121	1.781337496
H	4.331892126	-2.499041802	0.752578712	H	-4.641277483	-0.115623685	2.366872698
C	4.655930973	0.630259597	-2.192348962	C	-5.223491024	-0.055888316	-1.891881305
H	3.960023652	0.170158065	-2.919619402	H	-4.756986285	0.946126825	-1.945443309
H	5.653068310	0.249725904	-2.498600786	H	-6.313962962	0.153971210	-1.908577610

**Table S18:** Cartesian coordinates of the optimized geometry of the Isomers for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1:1}\text{-As}_4)(\text{Al}^t\text{Bu}_3)_2]$  at the B3LYP/def2- SVP level of theory.



As	0.109464812	1.793591151	0.012816721	As	-0.570980156	-0.115670125	-1.808159263
As	-1.225551574	0.084032309	-1.213839675	As	0.673235595	-1.012087452	0.159012070
Al	0.280202749	4.024749469	-1.914201949	C	-2.607934108	-3.028336640	2.644517703
C	-3.304126327	-2.162877552	2.239341521	C	-4.413306379	-1.901630878	-0.466487082
C	-1.456161204	0.580242674	4.041242675	H	-5.312342351	-1.586946927	-0.992420352
H	-0.962022103	0.983370468	4.922316731	C	-2.983994184	-2.465924218	1.266761072
C	-2.467752716	-0.930783939	2.607203362	C	-3.271284867	-2.516645984	-1.055070202
C	-2.081941680	1.339619254	3.012524998	C	-4.232209706	-1.854840597	0.943385777
C	-1.672775444	-0.802170769	3.785072684	H	-4.972805643	-1.505498161	1.660492182
H	-1.375294834	-1.618665314	4.440396396	C	-3.199229029	-3.078357336	-2.479123491
C	-2.399528316	2.835772806	3.081500072	C	-1.764681091	-3.463902306	-2.880687075

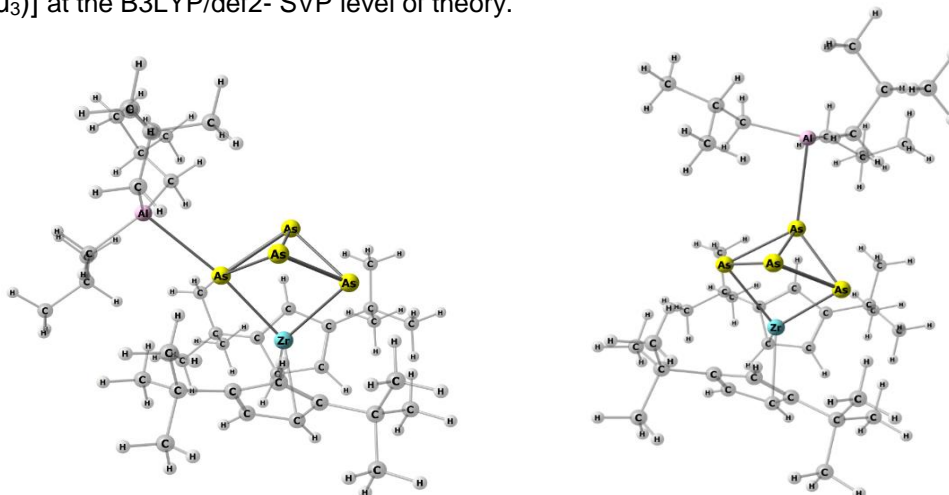


C	0.000000000	6.103775875	0.465828277
H	-0.220215704	5.280494485	1.171919592
C	-2.813414898	3.405307081	1.714223596
H	-2.005257229	3.326007552	0.972271346
H	-3.066682569	4.472145275	1.810452050
H	-3.699615035	2.893735596	1.308539489
C	-3.813441527	-2.127480870	0.787934054
H	-4.401725197	-1.220227024	0.580527704
H	-4.471876675	-2.990599481	0.603324491
H	-2.992969793	-2.177509065	0.059057280
C	0.821125348	5.526828103	-0.704232205
H	1.825803355	5.245395131	-0.331092067
H	1.035993754	6.353468319	-1.418268583
C	1.901163614	3.445582862	-2.955208254
H	2.604063293	4.288506503	-2.794897103
H	2.390385615	2.596588399	-2.435528589
C	-1.604527206	3.826114343	-2.578279285
H	-1.680765232	2.887751385	-3.163208204
H	-2.255677717	3.661093567	-1.698106349
C	-4.537548339	-2.122271840	3.182211329
H	-4.236527977	-2.172212884	4.240127997
H	-5.201940937	-2.976929520	2.974816737
H	-5.116890622	-1.197023994	3.038593894
C	-2.655740055	0.391406600	2.113416577
H	-3.235395892	0.650032929	1.230576509
C	-2.551516648	-3.481413125	2.487694972
H	-1.679241863	-3.586119988	1.827023246
H	-3.216793994	-4.336991114	2.293017192
H	-2.205979362	-3.568655525	3.529207817
C	-1.215424021	3.643760689	3.641086571
H	-0.923858295	3.300465320	4.646356177
H	-1.486038620	4.707717264	3.726386985
H	-0.336491386	3.573678894	2.985861497
C	-2.212031176	4.974889649	-3.419984738
H	-2.191835872	5.895258449	-2.806830970
C	-1.347775977	6.679635765	0.012274478
H	-1.200252763	7.495581257	-0.716937169
H	-1.915107858	7.097338916	0.861296712
H	-1.977592679	5.916107292	-0.468517256
C	-3.600750400	2.981366126	4.052610588
H	-4.473883998	2.415384843	3.692298467
H	-3.893783270	4.040275128	4.140822303
H	-3.350324549	2.611547155	5.059047998
C	-3.682854732	4.702801689	-3.772965066
H	-3.775543768	3.795344068	-4.395208956
H	-4.131362291	5.540353291	-4.334816317
H	-4.289176039	4.544369513	-2.865994267
C	3.277871399	3.036072841	-5.061365631
H	3.846903156	2.214785056	-4.590795984
H	3.844696313	3.967161369	-4.896472836
H	3.254255277	2.844721257	-6.148119659
C	-1.402329743	5.262630053	-4.691561011
H	-0.364437461	5.557052220	-4.460794380
H	-1.850885261	6.080336287	-5.279878268
H	-1.354609354	4.371973355	-5.341489063
C	0.791863476	7.164437533	1.248421324
H	1.744831483	6.757589236	1.624871981
H	0.223690028	7.547972821	2.113863610
H	1.034807439	8.025527559	0.601448394
C	1.862726777	3.128523165	-4.467502739
H	1.351411710	3.962292695	-4.984450924
C	1.073826900	1.850836148	-4.780165032
H	1.039784499	1.651684720	-5.864291419
H	0.035219107	1.911425562	-4.420532781
H	1.540335640	0.972853499	-4.299648240
Zr	0.000000000	0.000000000	2.076595048
As	-0.109464812	-1.793591151	0.012816721
As	1.225551574	-0.084032309	-1.213839675
Al	-0.280202749	-4.024749469	-1.914201949
C	3.304126327	2.162877552	2.239341521
C	1.456161204	-0.580242674	4.041242675
H	0.962022103	-0.983370468	4.922316731
C	2.467752716	0.930783939	2.607203362
C	2.081941680	-1.339619254	3.012524998
C	1.672775444	0.802170769	3.785072684
H	1.375294834	1.618665314	4.440396396
C	2.399528316	-2.835772806	3.081500072
C	0.000000000	-6.103775875	0.465828277
H	0.220215704	-5.280494485	1.171919592
C	2.813414898	-3.405307081	1.714223596
H	2.005257229	-3.326007552	0.972271346
H	3.066682569	-4.472145275	1.810452050
H	3.699615035	-2.893735596	1.308539489
C	3.813441527	-2.127480870	0.787934054
H	4.401725197	-1.220227024	0.580527704
H	4.471876675	-2.990599481	0.603324491
H	2.992969793	-2.177509065	0.059057280
C	-0.821125348	-5.526828103	-0.704232205

H	-1.090228643	-2.594181400	-2.889840000
H	-1.762469575	-3.894061020	-3.894733149
H	-1.334217328	-4.218037127	-2.204781601
C	-1.125503630	-3.430444270	2.731960957
H	-0.857406656	-4.177861350	1.969719945
H	-0.917368418	-3.879746040	3.715731017
H	-0.456334160	-2.567159265	2.613764604
C	-3.464388234	-4.310200145	2.825607920
H	-4.540913017	-4.079597268	2.809954799
H	-3.232420624	-4.791959054	3.789800057
H	-3.262996512	-5.037775073	2.024028946
C	-2.385258570	-2.816263507	0.021981927
H	-1.428166055	-3.319237703	-0.090774437
C	-2.941266582	-2.059637865	3.792663330
H	-2.334554219	-1.143467605	3.740047130
H	-2.735277131	-2.539967439	4.762316084
H	-4.002681614	-1.768459184	3.790735510
C	-3.770842785	-2.094615063	-3.516075913
H	-4.808638107	-1.808650212	-3.282536615
H	-3.778020889	-2.557589438	-4.515738288
H	-3.168866267	-1.177073509	-3.575569840
C	-4.066888140	-4.364288733	-2.486146123
H	-3.694541321	-5.097158153	-1.753511758
H	-4.043886979	-4.836201754	-3.482181840
H	-5.116500534	-4.142145865	-2.238182655
Zr	-2.668979688	-0.140401393	-0.046229956
As	-0.691809150	0.271784881	1.815119621
As	0.448820229	1.398746620	-0.097447870
Al	2.642184777	3.578308713	-0.433143789
C	-3.058661327	2.722762787	-2.722081117
C	-4.799596013	1.171629222	0.238364999
H	-5.640947187	0.653943364	0.694087200
C	-3.402681277	2.065080744	-1.378236652
C	-3.869639749	2.011838993	0.914065987
C	-4.505456580	1.188626364	-1.152708521
H	-5.090563589	0.693938173	-1.925677655
C	-4.036655349	2.554968984	2.336937565
C	2.707089118	2.457531514	-3.359050729
H	2.056378524	1.622837109	-3.034295202
C	-2.758873504	3.241118415	2.849169574
H	-1.910915546	2.542265577	2.906718071
H	-2.926722246	3.642419648	3.861042201
H	-2.460550132	4.085691818	2.209499237
C	-1.682314954	3.410720130	-2.710425009
H	-1.605670303	4.165020155	-1.921221835
H	-1.518349781	3.932874552	-3.666248568
H	-0.860978094	2.691968296	-2.582086609
C	2.461304437	3.656679340	-2.418225091
H	1.451499941	4.068892150	-2.611068605
H	3.143078486	4.483237311	-2.719609812
C	1.651529454	5.067153771	0.457136453
H	1.940961797	5.952049751	-0.148860148
H	0.563862241	4.964739087	0.263300174
C	4.112943653	2.609730712	0.507649206
H	3.907928305	2.624673180	1.595985279
H	4.081548397	1.540423838	0.226305786
C	-4.139990315	3.814776991	-2.942703145
H	-5.148458818	3.376073949	-2.997071578
H	-3.950887756	4.355136819	-3.884838693
H	-4.134631120	4.548846908	-2.121970341
C	-2.991592582	2.517006915	-0.090772173
H	-2.182364726	3.219779966	0.092146407
C	-3.121882117	1.735929817	-3.901599700
H	-2.334811500	0.970350168	-3.834025390
H	-2.977381739	2.275933493	-4.850744846
H	-4.094649085	1.224303975	-3.961747362
C	-4.454229090	1.455015159	3.328912545
H	-5.377379452	0.944931631	3.011147560
H	-4.648711217	1.891701475	4.321465503
H	-3.667004890	0.697365543	3.443671564
C	5.547049182	3.144110297	0.267436426
H	5.765164879	3.064077149	-0.814339973
C	4.155297126	1.955751798	-3.296379574
H	4.860396801	2.752093474	-3.593993278
H	4.315883900	1.101120248	-3.973919190
H	4.431262104	1.629744729	-2.281932977
C	-5.165777043	3.616389673	2.270612997
H	-4.912736585	4.421244948	1.562924391
H	-5.322667234	4.071434121	3.262472976
H	-6.118273691	3.169218080	1.946235101
C	6.600658707	2.302127190	1.002781642
H	6.442117415	2.342859905	2.094582566
H	7.624507726	2.660577105	0.799171805
H	6.548631905	1.243974531	0.700256629
C	1.297696610	6.760010169	2.335846264
H	0.204213169	6.781578217	2.181872248
H	1.732594656	7.566414436	1.722833337
H	1.489707808	7.002076216	3.395422124

H	-1.825803355	-5.245395131	-0.331092067	C	5.684650984	4.625327679	0.648578835
H	-1.035993754	-6.353468319	-1.418268583	H	4.995447264	5.267593344	0.072029095
C	-1.901163614	-3.445582862	-2.955208254	H	6.705776539	4.998468851	0.465164256
H	-2.604063293	-4.288506503	-2.794897103	H	5.460504889	4.781098379	1.718030561
H	-2.390385615	-2.596588399	-2.435528589	C	2.320470109	2.788075775	-4.809373626
C	1.604527206	-3.826114343	-2.578279285	H	1.266355373	3.102923062	-4.881429448
H	1.680765232	-2.887751385	-3.163208204	H	2.458981243	1.920493745	-5.477143810
H	2.255677117	-3.661093567	-1.698106349	H	2.939789924	3.614152354	-5.201376437
C	4.537548339	2.122271840	3.182211329	C	1.875997791	5.389257999	1.949337450
H	4.236527977	2.172212884	4.240127997	H	2.966874999	5.436146966	2.129748685
H	5.201940937	2.976929520	2.974816737	C	1.310583008	4.295818965	2.864502903
H	5.116890622	1.197023994	3.038593894	H	1.504060365	4.516156819	3.927569047
C	2.655740055	-0.391406600	2.113416577	H	1.747525731	3.308331963	2.645327804
H	3.235395892	-0.650032929	1.230576509	H	0.217411941	4.207886735	2.739461208
C	2.551516648	3.481413125	2.487694972	H	2.254464259	-1.557793213	2.986787245
H	1.679241863	3.586119988	1.827023246	C	3.219872525	-2.075717921	3.147578991
H	3.216793994	4.336991114	2.293017192	C	3.268911158	-3.304337310	2.210260332
H	2.205979362	3.568655525	3.529207817	Al	3.065383587	-3.180560153	0.229286886
C	1.215424021	-3.643760689	3.641086571	H	2.500234229	-4.030742418	2.538745664
H	0.923858295	-3.300465320	4.646356177	H	4.233192361	-3.830260574	2.382288309
H	1.486038620	-4.707717264	3.726386985	C	1.757622333	-4.475222996	-0.557883220
H	0.336491386	-3.573678894	2.985861497	H	0.806545832	-4.338227425	-0.006317716
C	2.212031176	-4.974889649	-3.419984738	H	1.532149384	-4.199117157	-1.606912546
H	2.191835872	-5.895258449	-2.806830970	C	4.300448541	-2.181659248	-0.976013989
C	1.347775977	-6.679635765	0.012274478	H	4.152091297	-2.586638036	-1.997499628
H	1.200252763	-7.495581257	-0.716937169	H	3.938916872	-1.136507474	-1.039872215
H	1.915107858	-7.097338916	0.861296712	C	5.813939040	-2.160330040	-0.659444987
H	1.977592679	-5.916107292	-0.468517256	H	5.948735514	-1.702889154	0.338282235
C	3.600750400	-2.981366126	4.052610588	C	4.332652564	-1.064015430	2.847321560
H	4.473883998	-2.415384843	3.692298467	H	5.327902014	-1.525688670	2.971986126
H	3.893783270	-4.040275128	4.140822303	H	4.282814990	-0.196893375	3.526172953
H	3.350324549	-2.611547155	5.059047998	H	4.272567091	-0.678301409	1.817553095
C	3.682854732	-4.702801689	-3.772965066	C	6.592806828	-1.296239098	-1.663090659
H	3.775543768	-3.795344068	-4.395208956	H	6.507003436	-1.707513269	-2.684193508
H	4.131362291	-5.540353291	-4.334816317	H	7.666242560	-1.245676137	-1.412041564
H	4.289176039	-4.544369513	-2.865994267	H	6.204569377	-0.265583870	-1.689545262
C	-3.277871399	-3.036072841	-5.061365631	C	0.953814860	-6.870670551	-0.938890527
H	-3.846903156	-2.214785056	-4.590795984	H	0.669723012	-6.662028027	-1.985317857
H	-3.844696313	-3.967161369	-4.896472836	H	0.064352989	-6.694644767	-0.311647459
H	-3.254255277	-2.844721257	-6.148119659	H	1.206076904	-7.942830120	-0.869033913
C	1.402329743	-5.262630053	-4.691561011	C	6.411986485	-3.572689554	-0.596767710
H	0.364437461	-5.557052220	-4.460794380	H	5.931111530	-4.189966221	0.182142482
H	1.850885261	-6.080336287	-5.279878268	H	7.490457445	-3.547342250	-0.368691708
H	1.354609354	-4.371973355	-5.341489063	H	6.289575564	-4.097183008	-1.560535992
C	-0.791863476	-7.164437533	1.248421324	C	3.261647486	-2.493972739	4.625673136
H	-1.744831483	-6.757589236	1.624871981	H	2.441041674	-3.188673652	4.869566385
H	-0.223690028	-7.547972821	2.113863610	H	3.177463149	-1.623771186	5.298965173
H	-1.034807439	-8.025527559	0.601448394	H	4.210389283	-3.007956071	4.860562000
C	-1.862726777	-3.128523165	-4.467502739	C	2.127631373	-5.978093474	-0.506697203
H	-1.351411710	-3.962292695	-4.984450924	H	2.363011631	-6.240672918	0.543472163
C	-1.073826900	-1.850836148	-4.780165032	C	3.372986930	-6.291871558	-1.347806066
H	-1.039784499	-1.651684720	-5.864291419	H	3.635165707	-7.361802496	-1.300275916
H	-0.035219107	-1.911425562	-4.420532781	H	4.255021844	-5.722071065	-1.012066449
H	-1.540335640	-0.972853499	-4.299648240	H	3.204289826	-6.036922744	-2.408578978

**Table S19:** Cartesian coordinates of the optimized geometry of the Isomers for [Cp<sub>2</sub>Zr(μ,η<sup>1:1</sup>-As<sub>4</sub>)(Al<sup>i</sup>Bu<sub>3</sub>)] at the B3LYP/def2- SVP level of theory.



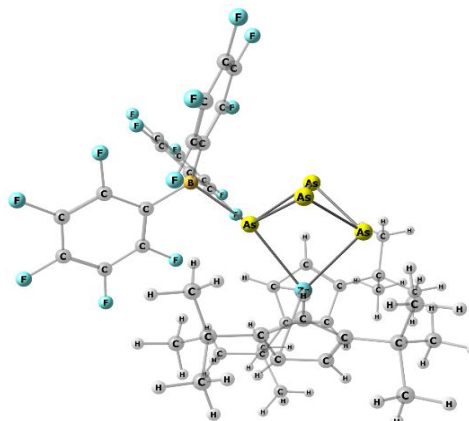
As	-1.860524802	-0.616148292	-2.145534620
As	0.160610311	-1.936888428	-1.526003022
C	-0.421565877	-2.422423461	3.045922279
C	-3.565271140	-0.679940652	1.908277090
H	-4.419564726	-0.028870009	2.081140554
C	-1.549417105	-1.768325392	2.238653342
C	-3.485879037	-1.711179070	0.928284117
C	-2.379828127	-0.700901034	2.694137309
H	-2.188964636	-0.073153370	3.562788436
C	-4.667958780	-2.272882421	0.129669195
C	-4.211570814	-3.246824718	-0.971275196
H	-3.565328318	-2.755907381	-1.714527069
H	-5.088191478	-3.647157282	-1.504784809
H	-3.661965741	-4.105408142	-0.555605610
C	0.429877809	-3.381106837	2.194728397
H	-0.176557676	-4.189588193	1.757690173
H	1.199698096	-3.855056666	2.823492820
H	0.944913152	-2.859351849	1.376274055
C	-1.122025528	-3.255531811	4.152814110
H	-1.718510488	-2.615002154	4.820961518
H	-0.372303929	-3.782620149	4.765554490
H	-1.795881821	-4.008981681	3.715860602
C	-2.220347598	-2.340539870	1.122012209
H	-1.855101338	-3.189136524	0.549043336
C	0.494244683	-1.390345831	3.724991550
H	1.054021727	-0.796552150	2.988441729
H	1.229717591	-1.901463647	4.365748167
H	-0.072080001	-0.698020865	4.366433303
C	-5.527844546	-1.161247886	-0.498100016
H	-5.887920824	-0.445953718	0.258238235
H	-6.415815189	-1.597004157	-0.983576265
H	-4.970237467	-0.600192926	-1.260623939
C	-5.542674104	-3.060695670	1.140184166
H	-4.962528227	-3.860211419	1.626834657
H	-6.399117371	-3.525852044	0.624702559
H	-5.937573525	-2.402457096	1.929625899
Zr	-1.732935156	0.218492275	0.436173906
As	0.950175248	-0.186958944	0.092709147
As	0.431088269	0.373719875	-2.289892162
Al	3.842047040	-0.399431938	0.112251451
C	-3.280753060	2.963409676	-1.970679121
C	-2.516232882	2.285266672	1.654701348
H	-2.821609965	2.160823386	2.691341348
C	-2.646516098	2.513080621	-0.646445721
C	-1.231548507	2.701704327	1.205971857
C	-3.371628870	2.149140502	0.527026444
H	-4.433042388	1.912170649	0.568925647
C	-0.130560587	3.296162199	2.087888103
C	3.907393519	0.811076103	3.039786384
H	2.826900070	1.038192797	2.962790153
C	1.213468542	3.391506440	1.346181910
H	1.582495699	2.403969796	1.032558938
H	1.977408859	3.836495960	2.001926598
H	1.141065960	4.026705981	0.450064076
C	-2.250359246	3.090951982	-3.106986992
H	-1.444290562	3.796153068	-2.851776725
H	-2.742913894	3.474641921	-0.414474795
C	-1.793226293	2.124188239	-3.359249927
C	4.222979415	-0.353128057	2.080362356
H	3.766767454	-1.280222379	2.481038076
H	5.315228907	-0.560215797	2.132563887
C	4.096073466	-2.288406137	-0.530480348
H	4.728556571	-2.730910328	0.266436444
H	3.139707606	-2.843782576	-0.444091450
C	4.161951467	1.194232086	-1.071726214
H	3.857589467	0.923263135	-2.102801445
C	3.451521273	1.988779967	-0.772085609
C	-3.865083025	4.375188943	-1.694378047
H	-4.644052314	4.342820827	-0.916853507
H	-4.315802391	4.787998469	-2.612031633
H	-3.080738300	5.070398914	-1.356628620
C	-1.317726774	2.790153134	-0.215705404
H	-0.506878389	3.109041134	-0.866178605
C	-4.431176097	2.048468081	-2.426760180
H	-4.069305987	1.047278913	-2.703174868
H	-4.923959117	2.479471896	-3.312780915
H	-5.200711240	1.933572450	-1.648294540
C	0.052720030	2.498293667	3.391295706
H	-0.881911843	2.442466298	3.971825463
H	0.805499675	2.983411121	4.032264453
H	0.393855499	1.473101400	3.192974149
C	5.579404932	1.813485373	-1.131070289
H	5.844711015	2.160917829	-0.115064759
C	4.664890155	2.094153255	2.674358442
H	5.755983019	1.929131335	2.714649373

As	-0.115236709	0.415268498	-1.855085918
As	0.443525807	-1.864121641	-1.003115775
C	-3.492005492	-3.304631855	0.864439755
C	-4.393221181	-0.005995000	-0.724437246
H	-5.002505081	0.892694158	-0.788541640
C	-3.495156975	-1.978751916	0.090107588
C	-3.673466302	-0.607690722	-1.797300360
C	-4.272101923	-0.830915773	0.427574508
H	-4.780931624	-0.664768494	1.375313773
C	-3.838286558	-0.267518866	-3.282207673
C	-2.730899380	-0.892188656	-4.149386433
H	-1.733253032	-0.512116309	-3.881667043
H	-2.904363634	-0.651951573	-5.210380674
H	-2.711211822	-1.989440762	-4.062573705
C	-2.422288553	-4.283080970	0.346611535
H	-2.563566019	-4.516388393	-0.720128727
H	-2.488061115	-5.233846441	0.898971417
H	-1.404153378	-3.890615245	0.479744182
C	-4.885685806	-3.942279995	0.618584264
H	-5.693395955	-3.307272349	1.014528673
H	-4.949505450	-4.924587335	1.115041907
H	-5.070027490	-4.090707953	-0.456920502
C	-3.094655672	-1.796902699	-1.264091437
H	-2.500884297	-2.506684413	-1.834829923
C	-3.311361477	-3.109710644	2.380184496
H	-2.305341481	-2.737147000	2.622919508
H	-3.443908519	-4.070507310	2.902742801
H	-4.048127589	-2.405416212	2.795576587
C	-3.877643417	1.251467114	-3.524711270
H	-4.676606716	1.738762731	-2.943714350
H	-4.073941877	1.461689254	-4.588221833
H	-2.923914209	1.726400097	-3.257678429
C	-5.197951597	-0.872167256	-3.720168438
H	-5.217687448	-1.961505982	-3.560237516
H	-5.375659308	-0.680880587	-4.791447350
H	-6.032623443	-0.432980680	-3.151995319
Zr	-2.026437829	0.281332716	0.094626351
As	-0.200440160	-1.307787031	1.355075808
As	1.431104894	0.082412404	0.085899821
Al	4.425244914	-0.164168646	0.318863041
C	-1.022390464	4.015843983	-0.640436861
C	-3.220404184	1.918867271	1.592097372
H	-4.195164584	1.620837433	1.972462152
C	-1.610769899	2.928812232	0.268642386
C	-1.978964708	1.791106282	2.279252540
C	-2.995103181	2.598687455	0.362886254
H	-3.769539686	2.906952904	-0.336783173
C	-1.817074084	1.467430610	3.768443316
C	4.305904734	2.971635160	0.429368081
H	3.222019593	2.917151351	0.210879161
C	-0.354994854	1.167537179	4.143010075
H	0.032275714	0.282151498	3.616778862
H	-0.276661407	0.972953773	5.224381492
H	0.308628469	2.015899957	3.915629591
C	0.515025705	3.981842863	-0.675488683
H	0.950672458	4.104999554	0.327573597
H	0.893713660	4.808508569	-1.297236697
H	0.897141168	3.043451127	-1.101762781
C	4.723563789	1.649252245	1.104158403
H	4.270878264	1.602429833	2.114571670
H	5.816829777	1.689933694	1.307528501
C	4.493520347	-1.559169693	1.747550661
H	5.316087867	-1.193094805	2.398021955
H	3.593888612	-1.470565699	2.389958792
C	4.742076600	-0.581572157	-1.610987941
H	4.427515746	-1.625847180	-1.804713133
H	4.061184334	0.039097422	-2.224682073
C	-1.460522921	5.369771735	-0.020666929
H	-2.557156471	5.468293267	-0.004460355
H	-1.050843674	6.208970544	-0.606739393
H	-1.097711506	5.468117104	1.014410333
C	-0.995225652	2.375722701	1.427708200
H	0.061468349	2.459055677	1.669679403
C	-1.563840947	3.945194306	-2.078819095
H	-1.237276718	3.026409815	-2.587593736
H	-1.191605134	4.801137781	-2.663979530
H	-2.663564332	3.982269549	-2.108130869
C	-2.707416922	0.290252504	4.205115100
H	-3.768281371	0.469427221	3.969117166
H	-2.636245969	0.143471310	5.294672011
H	-2.403547936	-0.647066970	3.719554715
As	-0.115236709	0.415268498	-1.855085918
As	0.443525807	-1.864121641	-1.003115775
C	-3.492005492	-3.304631855	0.864439755
C	-4.393221181	-0.005995000	-0.724437246

H	4.431006829	2.915382443	3.373106137	H	-5.002505081	0.892694158	-0.788541640
H	4.420109365	2.437868706	1.658230552	C	-3.495156975	-1.978751916	0.090107588
C	-0.588040391	4.733627438	2.449984775	C	-3.673466302	-0.607690722	-1.797300360
H	-0.736761397	5.342561546	1.544574784	C	-4.272101923	-0.830915773	0.427574508
H	0.172316713	5.230961483	3.074418474	H	-4.780931624	-0.664768494	1.375313773
H	-1.536377008	4.724165394	3.009517758	C	-3.838286558	-0.267518866	-3.282207673
C	5.622490702	3.044498464	-2.050477859	C	-2.730899380	-0.892188656	-4.149386433
H	5.377220645	2.765432243	-3.090353869	H	-1.733253032	-0.512116309	-3.881667043
H	6.620027917	3.517246310	-2.057766736	H	-2.904363634	-0.651951573	-5.210380674
H	4.892262410	3.806799813	-1.732584269	H	-2.711211822	-1.989440762	-4.062573705
C	5.132517989	-4.106151266	-1.989342499	C	-2.422288553	-4.283080970	0.346611535
H	4.244932302	-4.756266366	-1.892662022	H	-2.563566019	-4.516388393	-0.720128727
H	5.833290893	-4.383714221	-1.184786373	H	-2.488061115	-5.233846441	0.898971417
H	5.616115968	-4.342702603	-2.953152972	H	-1.404153378	-3.890615245	0.479744182
C	6.649543836	0.796965036	-1.551999416	C	-4.885685806	-3.942279995	0.618584264
H	6.703133775	-0.056642932	-0.854990279	H	-5.693395955	-3.307272349	1.014528673
H	7.652138875	1.255344338	-1.585029464	H	-4.949505450	-4.924587335	1.115041907
H	6.437266182	0.390067777	-2.555783748	H	-5.070027490	-4.090707953	-0.456920502
C	4.182786778	0.435107156	4.505184102	C	-3.094655672	-1.796902699	-1.264091437
H	3.608979318	-0.456887743	4.805688393	H	-2.500884297	-2.506684413	-1.834829923
H	3.919927833	1.253963741	5.197608939	C	-3.311361477	-3.109710644	2.380184496
H	5.252042735	0.203240549	4.653941547	H	-2.305341481	-2.737147000	2.622919508
C	4.734194478	-2.623991647	-1.897321025	H	-3.443908519	-4.070507310	2.902742801
H	5.664540290	-2.034306515	-2.000055205	H	-4.048127589	-2.405416212	2.795576587
C	3.827267034	-2.246973802	-3.075538901	C	-3.877643417	1.251467114	-3.524711270
H	4.309278980	-2.464657754	-4.043612056	H	-4.676606716	1.738762731	-2.943714350
H	3.566036013	-1.177250609	-3.065707020	H	-4.073941877	1.461689254	-4.588221833
H	2.882452055	-2.817756851	-3.041505644	H	-2.923914209	1.726400097	-3.257678429

**Table S20:** Cartesian coordinates of the optimized geometry for  $[\text{Cp}''_2\text{Zr}(\mu, \eta^{1:1:1}\text{-As}_4)(\text{B}(\text{C}_6\text{F}_5)_3)]$  at the B3LYP/def2- SVP level of theory.

Zr	2.490684707	-0.231908978	0.090899804
As	2.379599655	2.225005194	-1.154775720
As	0.265911360	2.669075850	0.105223132
As	-0.263009465	0.235677654	-0.089055036
As	0.174483336	1.607780323	-2.112172926
F	-0.896871250	-1.748379114	-2.111394067
F	-5.259108590	-0.448143953	-0.756037859
F	-3.469502870	1.515032469	-2.417197063
F	-2.538968988	1.776920681	2.235930619
F	-1.947105529	-3.237601460	-4.028158101
F	-4.303637215	4.030327193	-2.375474919
F	-1.150339146	-2.517547083	0.768904687
F	-4.785124539	0.308759421	1.960560135
F	-4.659989947	-3.384738676	-4.366390725
F	-6.297477979	-1.966171436	-2.698500873
F	-3.379600465	4.302841269	2.245706994
F	-4.278937581	5.473443326	-0.056241641
F	-5.353407828	-1.303618009	3.983704916
F	-1.737045376	-4.108413324	2.818990029
C	-3.025085703	-0.987574940	-1.337953494
F	-3.855899016	-3.535486732	4.460463438
C	-4.407614247	-1.115611175	-1.547919337
C	-2.243187454	-1.745501554	-2.209816987
C	3.183734026	-2.677775789	-0.555168086
C	-2.763510362	-2.547822292	-3.230420001
C	-3.006937701	2.274123109	1.079298773
C	-4.976296255	-1.899642880	-2.551443627
C	-4.143066205	-2.627178242	-3.404019720
C	-3.428516425	3.602788236	1.113563507
C	-3.034659694	1.467054338	-0.069965732
C	-2.892618752	-0.976223988	1.278263624
C	-3.462696274	2.135086962	-1.228065865
C	-3.881259661	4.205491726	-0.060959107
C	4.364633254	-0.225249051	1.739081576
H	5.323044008	-0.614900698	1.402412729
C	4.003400380	1.152333329	1.823669802
C	2.696555850	1.184562214	2.391222282
H	2.131854350	2.090367293	2.598402059
C	-2.193411116	-2.158730289	1.550563239
C	-3.981404074	-0.743513466	2.134443001
C	-3.896859298	3.464107034	-1.240992067
C	4.978398576	2.333513629	1.745082515
C	3.589978945	-1.033298331	-2.173065876
C	5.938068518	2.228892901	0.548260947
H	6.465371738	1.262320863	0.525353406
H	6.703263371	3.019008885	0.607269042
H	5.406044613	2.351733985	-0.404501135
C	4.163161097	-1.795193113	-1.102266579
H	5.223796349	-1.816038913	-0.858622303
C	3.317474575	-1.004219470	2.312289838
H	3.350597287	-2.074743028	2.481124522
C	4.390598865	-0.371789981	-3.302514104
C	2.286854854	-0.127423198	2.758398536



C	4.251411204	3.689631175	1.700006556
H	3.616265205	3.788270206	0.807208621
H	4.989199613	4.507117525	1.676356736
H	3.620443732	3.846262275	2.588475578
C	2.211115053	-1.367867646	-2.192912277
H	1.466964553	-0.991046988	-2.888544235
C	3.463102857	-3.993639890	0.183034823
C	5.814384131	2.275143135	3.051751293
H	5.166888406	2.328907290	3.940729505
H	6.518245277	3.122593977	3.090244022
H	6.398459233	1.343960159	3.115197471
C	2.319409585	-4.397452805	1.131300222
H	2.217404246	-3.710733023	1.980889183
H	2.503037032	-5.404876189	1.537030124
H	1.347868408	-4.424127530	0.615291946
C	-2.483768254	-3.023803289	2.604273879
C	-3.557261931	-2.731322266	3.444888867
C	-4.313643782	-1.584966216	3.201911132
C	5.070768893	-1.530214284	-4.079086077
H	5.784626748	-2.078202747	-3.444822582
H	5.623340561	-1.133038723	-4.946220990
H	4.325003900	-2.250371681	-4.450314998
C	1.955434747	-2.350894250	-1.197467762
H	0.992919503	-2.831126868	-1.036307455
C	4.805935630	-3.980626840	0.938092290
H	5.652541620	-3.805511981	0.256240160
H	4.973495198	-4.958372778	1.416293455
H	4.846979120	-3.217244361	1.727416027
C	3.480827469	0.390071388	-4.282765014
H	2.730362984	-0.271872195	-4.741761570
H	4.086144042	0.814726023	-5.099080353
H	2.952187261	1.220890253	-3.793414306
B	-2.553218477	-0.082728698	-0.051304302
C	1.202609703	-0.475413481	3.781352579
C	3.563618647	-5.072406930	-0.930449378
H	2.616910489	-5.163035593	-1.484160279
H	3.797009155	-6.055097442	-0.488767985
H	4.356541266	-4.825501552	-1.653430296
C	1.848922686	-0.253813587	5.174874833
H	2.139755814	0.798518187	5.317134474
H	2.749115465	-0.875345653	5.301937350
H	1.134390268	-0.520218858	5.970745054
C	5.482639686	0.576967310	-2.780658319
H	5.043528770	1.469128936	-2.312523020
H	6.119614521	0.916633105	-3.612844720
H	6.136837388	0.087725087	-2.042212264
C	-0.032072063	0.430958786	3.668034658
H	-0.732769162	0.218838297	4.490581111
H	-0.573327766	0.269108678	2.727777207
H	0.225519173	1.499204137	3.728891211
C	0.771016342	-1.947119203	3.673653832
H	1.602302952	-2.632859896	3.897759582
H	0.388997814	-2.187536148	2.672241510
H	-0.026542699	-2.163939341	4.400604649

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